

Nabisab Mujawar Mubarak
Mahmood Anwar
Sujan Debnath
Izman Sudin

Fundamentals of Biomaterials

A Supplementary Textbook

Nabisab Mujawar Mubarak, Mahmood Anwar, Sujan Debnath and
Izman Sudin

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Nabisab Mujawar Mubarak
Petroleum and Chemical Engineering, Faculty of Engineering, Universiti
Teknologi Brunei, Bandar Seri Begawan, Brunei Darussalam

Mahmood Anwar
Department of Mechanical Engineering, School of Computing, Engineering
and Built Environment, Glasgow Caledonian University, Glasgow,
Scotland, UK

Sujan Debnath
Department of Mechanical Engineering, Curtin University Malaysia, Miri,
Malaysia

Izman Sudin
Department of Materials, Production and Industrial Engineering, Faculty of
Mechanical Engineering, Universiti Teknologi Malaysia, Johor Bahru,
Malaysia

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In the name of Allah, the Most Gracious and the Most Merciful. First of all, I would like to raise my heartfelt gratitude and appreciation to Allah S.W.T for the permission, guidance, wisdom and blessing for all these years till now, when I have reached this important destination of my journey in life to accomplish my goal. Finally, I would like to present my most heartfelt and warmest appreciation to the great parents and parents-in-law (may Allah SWT bless and reward them), brothers and sisters who always encouraged and supported me during the completion of the book. Special and heartiest gratitude to my dearest wife, Muna Tasnim Mukhtaruddin, and kids, Muhammad Fayyad, Muhammad Fawwaz and Mulaika Faleeha, for their invariable encouragement endless sacrifices, patience, understanding, ideas and inspiration from time to time in finishing the book smoothly and timely.

Dr. Nabisab Mujawar Mubarak

This book would not have been possible without sacrifices from the family. I dedicate this book to my beloved mother, Mrs. Rubina Yeasmin, whose dream and patience lead to achieving my academic path.

Dr. Mahmood Anwar

This book would not have been possible without sacrifices from the family. Thanks to my, wife, daughter and children.

Dr. Sujan Debnath

This book would not have been possible without sacrifices from the family. I dedicate this book to my loving wife and my lovely daughters.

Prof. Dr. Izman Sudin

Preface

Realizing the difficulty of grasping the vast field of biomaterials as a new learner, this book has presented information on various fundamental concepts incorporating modern physics, materials science, and medical biology in a simple question-and-answer format to help the students. The objective of this book is to make a smooth transition for any students from different disciplines entering to biomaterials field require a strong background in materials science prior knowledge and Authors have found such need from their prolonged academic experience with the students entering to biomaterials arena and found them always struggle to begin. During preparing the manuscript, emphasis has been given to fundamental materials science and engineering knowledge, including atomic physics. Chapters 2 to 7 are written, including compiled data for tables and redrawn schematics based on the references B. L. Theraja, 2000, "Modern Physics", S.Chand & Company Ltd. New Delhi, India, A. Pytel & F. L. Singer, 1995, "Strength of Materials", Haper & Row, New York, USA, J. P. Schaffer, A. Saxena, S. D. Antolovich, T. H. Sanders, and Steven B. Warner, 1999, "The Science and Design of Engineering Materials", WBC/McGraw-Hill, USA, Sydney H. Avner, 1997, "Introduction to Physical Metallurgy", Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, "Foundations of Materials Science and Engineering", 2004, McGraw-Hill, 3 Ed, New York, USA and William D. Callister Jr. & David G. Rethwisch, 2009, "Materials Science and Engineering: An Introduction", 8th ed. John Wiley and Sons. NJ, USA. Chapter 8 is written based on the references J. P. Schaffer, A. Saxena, S. D. Antolovich, T. H. Sanders, and Steven B. Warner, 1999, "The Science and Design of Engineering Materials", WBC/McGraw-Hill, USA, A.S. Khanna, 2002, "Introduction to High-Temperature Oxidation and Corrosion", ASM International, USA, Mars. G. Fontana, 1987", Corrosion Engineering", McGraw-Hill, 3 Ed, Singapore, Sydney H. Avner, 1997, "Introduction to Physical Metallurgy", Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, "Foundations of Materials Science and Engineering", 2004, McGraw-Hill, 3 Ed, New York, USA and William D. Callister Jr. & David G. Rethwisch, 2009, "Materials Science and Engineering: An Introduction", 8th ed. John Wiley and Sons. NJ, USA. Chapters 12 to 14 are written, including compiled data for tables and redrawn schematics based on the reference W. K. Ovalle and P.C. Nahirny,

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Last but not least, no academic work is error-free despite providing the best effort to avoid any errors. Hence, we welcome any feedback, suggestions, queries, and corrections you may wish to contribute to this first edition, and kindly do not hesitate to contact us.

Dr. Nabisab Mujawar Mubarak

Dr. Mahmood Anwar

Dr. Sujan Debnath

Prof. Izman Sudin

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Dr. Nabisab Mujawar Mubarak

I would like to take this opportunity to express my sincere gratitude to the Department of Mechanical Engineering, School of Computing, Engineering and Built Environment, Glasgow Caledonian University, Glasgow, Scotland, UK, and colleagues in the Mechanical Engineering Department of Curtin University, Malaysia Campus, for the continuous support and encouragement at all times. I would also like to express my heartiest gratitude to Dr. Engku Mohammad Nazim Bin Engku Abu Bakar from University Teknologi Malaysia and Associate Professor Dr. Ian J. Davies from Curtin University, Perth Campus, for their various feedbacks on the Materials Science and Engineering aspects during manuscript preparation. My special thanks go to all my co-authors and editors for their valuable contributions.

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Dr. Sujan Debnath

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Prof. Dr. Izman Sudin

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About the Authors

Dr. Nabisab Mujawar Mubarak is Associate Professor at the Faculty of Engineering, Universiti Teknologi Brunei, Brunei Darussalam. He serves as a scientific reviewer in numerous Chemical Engineering and Nano Technology journals. In research, Dr. Mubarak has published more than 270 journal papers, 30 conference proceedings and authored 30 book chapters, and the H-index is 54. His interest areas are carbon nanomaterials synthesis, magnetic biochar production using microwave and wastewater treatment using advanced materials. He is a recipient of the Curtin Malaysia Most Productive Research Award, Outstanding Faculty of Chemical Engineering Award, Best Scientific Research Award London and an exceptional scientist in publication and citation by i-Proclaim, Malaysia. He also has the distinction of being listed in the top 2% of the world's most influential scientists in chemicals and energy. The *List of the Top 2% Scientists in the World* compiled and published by Stanford University is based on their international scientific publications, a number of scientific citations for research and participation in the review and editing of scientific research. Dr. Mubarak is Fellow Member of the Institution of Engineers, Australia, Chartered Professional Engineer (CPEng) of the Institution of Engineers, Australia, and Chartered Chemical Engineer of the Institute of Chemical Engineering (IChemE), UK. He has published four books and is Co-editor for ongoing Elsevier-edited books: (1) *Nanomaterials for Carbon Capture and Conversion Technique*, (2) *Advanced Nanomaterials and Nanocomposites for Bioelectrochemical Systems*, (3) *Water Treatment Using Engineered Carbon Nanotubes* and (4) *Emerging Water Pollutants: Concerns and Remediation Technologies*.



Research 5) Hybrid Nanomaterials for Sustainable Applications 6) Sustainable Nanotechnology for Environmental Remediation 7) Nanotechnology for Electronic Applications-Production 8) Nanotechnology for Biomedical Applications 9) Contemporary Nanomaterials in Material Engineering Applications Interests: Advanced carbon nanomaterials

synthesis via microwave technology, MXene synthesis and its application in wastewater treatment and energy storage, graphene/CNT buckypaper for strain sensor application, biofuels, magnetic buckypaper, immobilization of enzymes, protein purification, magnetic biochar production using a microwave and wastewater treatment using advanced materials.

mubarak.mujaawar@utb.edu.bn

Dr. Mahmood Anwar is Lecturer at the Department of Mechanical Engineering, Glasgow Caledonian University, Scotland, UK, and previously about 8 years in Curtin University, Sarawak Campus, Malaysia. Prior to join academic position, he was Research Scientist in Hitachi CFP PTE., Singapore, and involved as Scientist for High Voltage Component Research and Corrosion Protection projects. He was also a technical adviser of several palm oil industries for acoustic materials design. He has been a long-serving member of IMM Coating Fingerprint Task Force for Coating Standard Development toward Oil and Gas industry and led the Committee of Standard Development in IMM as Co-chair. He is also a professional certified coating quality controller for Oil and Gas Industry. He has published more than 30 research papers up to date comprising international journals and conferences including regular reviewer of several international journals. He is very active in industrial research and academic accreditation works, serving as an auditor for numerous academic programs. Due to his industrial research contribution, he has been awarded Fellow of Institute of Materials, Malaysia. He is Chartered Engineer (CEng MIMMM) and Senior Fellow of the Higher Education Academy (SFHEA), UK, and Member of ASME and TMS, USA.



Mahmood.Anwar@gcu.ac.uk

Dr. Sujan Debnath (CEng MIMechE, SFHEA) is Associate Professor in the Department of Mechanical Engineering at Curtin University Malaysia. Dr. Debnath obtained his Ph.D. degree from the University of Science Malaysia majoring in applied mechanics and heat transfer with specific research focusing on interfacial thermal mismatch stress analysis in electronic packaging. He served as HOD of Mechanical Engineering from 2014 to 2017 at Curtin Malaysia. Over the years, Dr. Debnath dedicated his research in the areas of mechanical engineering especially on polymer biocomposites and nano-composites, sustainable metal cutting, nano-enhanced Minimum Quantity Lubricant (MQL) machining, folding design using origami principle and thermal management in electronic packaging. He has published more than 120 international journal papers and authored one book and five book chapters. His current research H-index is 27. Dr. Sujan has delivered 15 keynote speeches at international conferences and organized and/or chaired 10 international conferences. Dr. Sujan is Chartered Professional Engineer with the Institute of Mechanical Engineering, UK (CEng MIMechE), and Senior Fellow (SFHEA) of the Higher Education Academy, UK. Dr. Sujan is a registered Level 1 supervisor at Curtin University for doctoral and master's theses.



Prof. Dr. Izman Sudin is Professor at the Faculty of Mechanical Engineering, Universiti Teknologi Malaysia, Johor, Malaysia. He is one of the Malaysian prolific academics and pioneer in biomaterials research, particularly in Bio-Manufacturing. In this 35 years of academic career, he has supervised 60 postgraduates research students among them 30 Ph.D. graduates, published more than 137 journals, has an H-index of 21 and led 14 research grants as a principal investigator.



izman@utm.my

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1. Introduction

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

1.1 What Are Biomaterials

As human civilization advanced, the study of biomaterials also developed, incorporating various materials at various length scales, from nano to macro, with the straightforward goal of extending and improving human life. Silver was utilized as an antibacterial agent to fight infection over a thousand years ago. Even in the earliest periods of civilization, several surgical techniques were used. However, from 1901 to 2000, biomaterials saw arguably the most important advancements. Over the past 60 years, artificial joints have enhanced millions of people's quality of life, resorbable sutures have sped up surgical procedures, and various cardiovascular devices have prevented millions of deaths, to mention a few. The development of tissue engineering and organ regeneration is pushing the boundaries of science and will increase the excitement of the years 2001–2100 in the field of biomaterials. To fully enjoy the benefits, however, competent engineering design, suitable materials, and device characterization are also required. They are just as vital as the design of biomaterials.

Additionally, it's critical to conduct testing following relevant standards to obtain regulatory approval before commercializing a biomedical device. Overall, the advantages of biomaterials research can only be realized when these materials are thoroughly defined at the materials and device levels while adhering to regulatory guidelines. It is difficult to conduct a wide range of tests using various approaches, given the multidisciplinary character of the topic. Realizing the difficulty to grasp on the vast field of biomaterials being new learner. This book has presented information on various fundamental concepts incorporating modern physics, materials science and medical biology in a simple question and answer format in order to help the students. The objective of this book is to make smooth transition for any students from different discipline entering to biomaterials field required strong background of materials science prior knowledge and Authors have found such need from their prolong academic experience with the students entering to biomaterials arena and found them always struggle to begin. During preparing the manuscript, emphasis has been given to fundamental materials science and engineering knowledge including atomic physics. Chapter 2 to 7 are written including compiled data for tables and redrawn schematics based on the references B. L. Theraja, 2000, "Modern Physics", S.Chand & Company Ltd. New Delhi, India, A. Pytel & F. L. Singer, 1995, "Strength of Materials", Haper & Row, New York, USA, J. P.

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1.2 What Are Types of Materials

Materials can be divided into groups based on their macrostructures, bonding, and crystal structure. Each subgroup of materials has some characteristics in common, so it is possible to evaluate the performance of these materials in various applications by grouping them. Materials can be grouped into three major categories: metals, ceramics, and polymers when it comes to bonding kinds. Metals are substances that are joined together by

metallic bonds. Metals exhibit malleability in their mechanical characteristics and are both thermally and electrically conductive due to the abundance of free electrons in their metallic bonds. Ceramics are substances that are predominantly ionized and covalently bound. Ceramics are typically non-conducting materials thermally and electrically because ionic and covalent bonding does not supply free electrons. However, certain ceramics exhibit conductivity at greater temperatures due to the movement of flaws. Polymers are substances built on lengthy carbon chains and are covalently bonded with some secondary bonding, with the “mers” or units being connected across a considerable distance. The majority of polymers lack conductivity because of covalent bonding. A new class of materials known as composites is created when three of these primary materials are combined without sacrificing their original properties. Wood and bone are two examples of natural composites. Materials can be divided into three classes based on their unit cells, which are the fundamental building blocks of all substances: crystalline, semicrystalline, and amorphous. Iron, titanium, chromium, or polycrystalline ceramics are crystalline materials because they replicate the unit cell in all three directions and preserve long-range order. The Bravais lattice of the unit cell is defined by its basic three-dimensional shape and atom positions, which can be, for instance, body-centered cubic, face-centered cubic, or hexagonal close-packed (hcp). “Cubic” or “hexagonal” refer to crystal systems defined by the shape of the unit cell, respectively, and “body-centered” or “face-centered” refers to specific atom positions. These straightforward structures are typical of most crystalline metallic systems, which make up most metallic systems. Many materials only exhibit short-range repetition of the unit cell, which does not repeat itself in three dimensions for extended distances. Amorphous materials, also called glass, are substances with the short-range ordering of unit cells. Glassy materials exhibit unusual features like glass transition temperature (T_g) when a liquid phase changes into a solid rubbery phase since they lack ordering. Another class of substances includes those that are both partially crystalline and partially glassy. These substances are referred to as semicrystalline substances. Numerous polymeric materials, among others, exhibit a semicrystalline character. Materials can also be divided into natural and synthetic categories. Natural materials are those that can be found in nature, such as bones, coral, rocks, and wood. Ceramics, polymers, and their composites are the most common natural materials. These

materials were created by Mother Nature to serve a range of functions, including those of sensors, reservoirs, structural support, and energy converters. Most of these materials have intricate chemistry and structures, which humankind is still studying to increase its income. Synthetic materials are manufactured by humans and have a specific purpose. These materials include ceramics for bone tissue engineering and metallic ones like steel for fracture management devices, titanium and its alloys for implants, polymers for ocular lenses, and steel for fracture management devices. Synthetic materials are designed to have particular chemistry and structural characteristics that can be used to enhance our daily lives. Depending on the application, it may be necessary to determine the materials' physical, chemical, mechanical, and, occasionally, biological properties after processing. Additionally, materials can be categorized according to their macrostructures, such as dense or porous. Most natural materials, including rocks, tissues, and wood, are porous. These materials' porosity can be used for a number of things. The majority of ceramic materials still have porosity. Porosity can vary in size and distribution and be nonuniform. Materials' porosity can range from 1 to 10%, as in the case of cortical bone, to as much as > 70% in some cancellous bones. These materials are lighter in weight and frequently exhibit nonuniform characteristics in different directions because of their porosity. However, it is very challenging to replicate the composition, structure, and characteristics of such natural materials. Materials that exhibit no porosity are referred to as dense materials. Most metallic materials are naturally dense, with only 1% remaining porosity. Dense materials can be easily moulded using various forming techniques because they are often isotropic. Different kinds of materials are depicted schematically in Fig. 1.1. Additionally, any substance may fit under several of these categories. For instance, bone is a porous, natural substance made of ceramic and polymers.

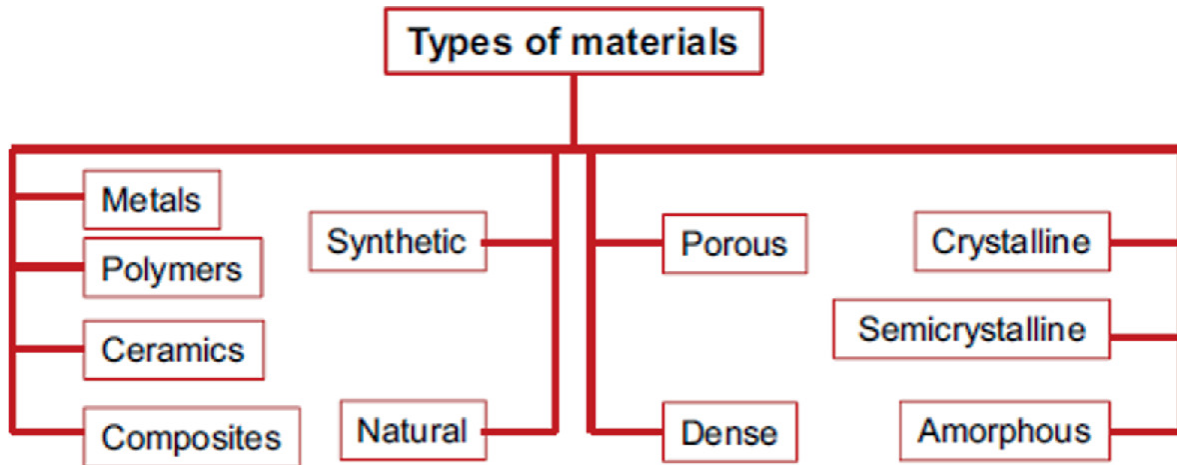


Fig. 1.1 Types of materials

1.3 Biomaterials and Biocompatibility

A biomaterial is a synthetic or natural substance that has a biological function or can be utilized to substitute a body part or tissue in medical applications. A biomaterial is created to interact with other biological systems. It can also be used to administer a biological agent or a medication. Based on the demands of the application, biomaterials are created. The Romans, Aztecs, and Chinese employed gold in dental applications at the dawn of civilization. Dental implants made of seashells were discovered to have been used by the Mayans, and tests showed that the implants integrated with the bone. A biomaterial must be biocompatible or friendly to biological systems and not harmful to them at any level, including at the cellular or system level. A biocompatible substance must elicit the proper host response or be able to carry out its intended function in a given application without causing negative side effects. This novel paradigm calls for the knowledge and integration of ideas from many diverse domains, including but not limited to chemistry, biology, materials science, mechanical, chemical, and electrical engineering, as well as medicine. Biomaterials supplement, repair, or replace any body part that has suffered damage through an accident, illness, or injury. The use of autografts, or tissue or organ transplants from the same person to another, is a common procedure in modern medicine for tissue regeneration. However, their use is constrained by their restricted accessibility, donor site morbidity, and, most importantly, the requirement for a second operation. The use of allograft, or a tissue or organ transplant from a donor of the same species as

the recipient, is an alternative that is possible. The other option is xenograft, which is the transplantation of an organ or tissue from a donor who is a different species from the recipient. Due to the immunogenic reaction and potential for negative biocompatibility in patients' bodies, the use of both allografts and xenografts is relatively constrained. These factors highlight the biomaterials that can be obtained from various sources, whether they be synthetic or natural. Modern biomaterials and their future uses didn't start to take shape until the turn of the twentieth century.

The primary goals of these first-generation contemporary biomaterials are biocompatibility and fundamental functionality. Metal plates have supported lengthy bone fractures since the early 1900s to promote quicker and more effective healing. The 1930s carried out full joint replacement surgeries with various successes. The development of synthetic heart valves (a metal cage enclosing a silicone elastomer ball) and total hip arthroplasty systems were made possible by the invention and widespread use of synthetic plastics (ultrahigh molecular weight polyethylene). The desk-sized pacemaker and intraocular lenses made of poly(methyl methacrylate) PMMA are two more significant inventions from this period. Beginning in the 1960s, new biomaterials emerged due to growing knowledge of biology's complexity. Materials were first created by scientists and engineers expressly for biomedical applications.

Materials that were just bio-compatible started to lose importance as attention shifted to technologies that accounted for the unique requirements of each biological system. During this time, numerous bioresorbable materials—biomaterials reabsorbed in biological systems—were also developed. The development of synthetic polymers like Teflon, still widely employed in various surgical and vascular grafting procedures, was one of the most significant contributions to the field of materials science. Hydrogels influenced the development of soft contact lenses. Poly (lactic-glycolic acid) (PLGA) was created for resorbable sutures.

The development of plastic materials was not the only innovation at this time. Additionally, ceramics like calcium phosphate-based synthetic bone analogues were produced. Today, synthetic materials are employed more frequently than allografts or autografts, which remove bone from a different part of the patient's body (processed cadaver bones). Traditional stainless steel orthopedic implants were replaced with lighter titanium alloys with improved biocompatibility.

1.4 What Are the Different Types of Biomaterials

Biomaterials can be divided into four main types, just like other materials: (1) polymers, (2) metals, (3) ceramics, and (4) composites, as in Fig. 1.2. The most common type of biomaterials are polymers, which can be applied to both soft and hard tissues. Polymers are frequently employed in applications for medication delivery. Polymers can be synthetic (like silicone rubber, PMMA, poly(vinyl chloride), and co-PLGA) or natural (like collagen, sodium alginate, and cellulose). Metals are mostly used in orthopedic and dentistry applications. Ti, stainless steel, and Co-Cr alloy are the most often utilized metals. Ceramics are mostly used in non-load-bearing applications or as coatings on metal implants for usage in hard tissue repair, regeneration, and augmentation. Bioglass, calcium phosphates (CaP), and alumina (Al₂O₃) are ceramic biomaterials most often utilized. The majority of composite biomaterials are composed of polymer-ceramic composite.

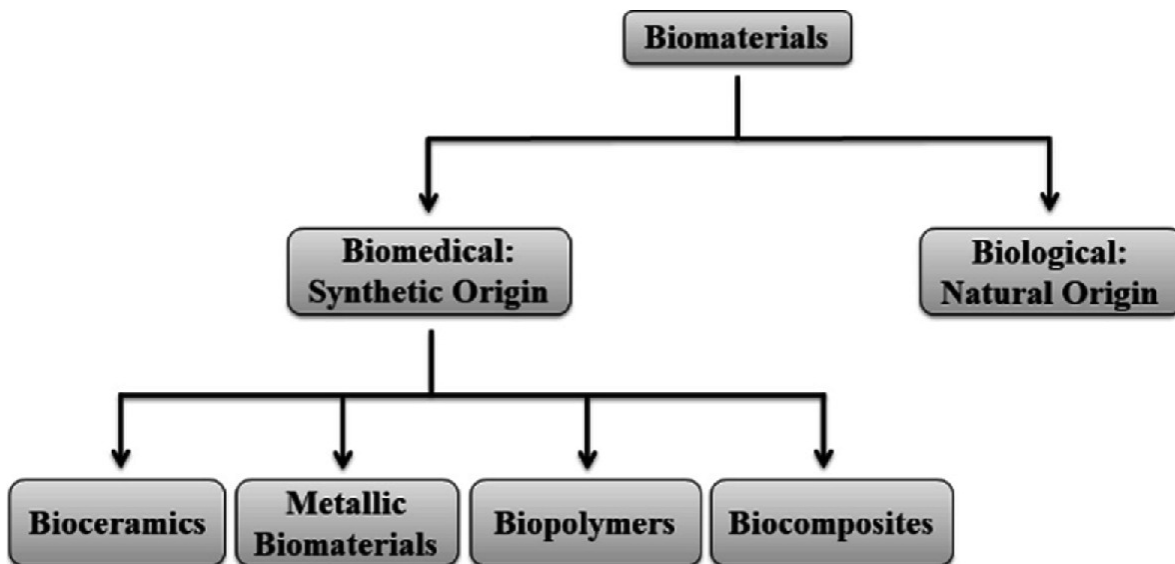


Fig. 1.2 Biomaterial classification

There are four different categories of responses between biomaterials and tissues. (1) Toxic: Materials that are toxic kill nearby tissue. (2) Bioinert: Nontoxic but physiologically inactive substances can elicit this reaction. In vivo, fibrous tissue encapsulation of the bioinert substance results in the implant becoming loose and eventually failing. Most frequently, this occurs with metallic implants. A metallic implant with a

bioactive substance covering may stop fibrous tissue encapsulation. (3) Bioactive: If a substance is nontoxic and physiologically active, a reaction of this kind will be observed. The phrase “biologically active” denotes forming an interfacial bond between the substance and the host tissue. This group includes the majority of calcium phosphate ceramics, bioactive glasses, and various types of polymers. (4) Bioresorbable: When a harmless substance dissolves in vivo, such as calcium sulphate (plaster of Paris), tricalcium phosphate, bioactive glasses, and PLGA, this type of reaction is observed. As a result, the synthetic material can be replaced by the host tissue around it.

1.5 Basic Properties of Biomaterials

There are several excellent books on material characteristics. This concise introduction to material properties solely familiarizes the reader with the topic. The most crucial material characteristics for biomaterials in connection to their surface and bulk qualities are chemical, physical, mechanical, and biological. Chemical attributes have to do with a material's chemistry, including its composition, bonds, and atomic structure. Physical characteristics deal with phases, density, and various kinds of porosity. Mechanical characteristics cover materials' strength, toughness, hardness, and various failure causes. The behavior of materials in a biological context is the subject of biological properties. In vitro qualities are those that are tested in a biological environment that is established in a Petri dish; in vivo properties are those that are measured inside an animal or human body. Surface properties deal with the characteristics of materials at the surface where all bonds are broken. The surface properties of materials are frequently very different from their bulk properties due to dangling bonds. Materials chemistry, structure, and processing are all related to these material characteristics. For instance, carbon is a substance with a wide range of properties based on its bonding and structure. Diamond, the hardest substance known to man, is made when carbon atoms are tightly packed and completely covalently bonded. Conversely, graphite is created when carbon forms an hcp structure with covalent bonds and some secondary bonding. Graphite is a delicate substance. As a result, materials' qualities cannot be determined just by their chemistry. Similarly, materials processing will significantly affect a material's qualities and performance

even though its chemistry and structure are the same. Strength ratings for a ceramic body made of highly pure calcium phosphate might vary greatly depending on the residual porosity of the part, which is directly related to the production conditions. To comprehend a material's qualities, one must thoroughly understand its structure and processing. Reviewing the benefits and drawbacks of various material systems is crucial in this context. These general characteristics merely direct the selection of materials for a given application. The fundamental benefit of a metallic system is its ductility. Due to its lengthy history, the field of metallurgy is extremely rich. Metallic materials may be processed dependably due to thousands of years of knowledge and their high strength and durability. These substances are widely accessible and naturally conductible. Naturally, metallic materials make up the majority of substantial industrial structures. Metals are frequently employed in bone fracture repair and joint replacement. Metallic materials resist corrosion and offer great strength and fracture resistance. Ceramics often have a lower in vivo wear rate and are harder than metals. Ceramics are strong in compression and immune to microbiological attacks. Bioglasses, calcium phosphates, zirconium, and aluminum oxide are ceramic biomaterials most often utilized. The last two are employed as bioactive and bioresorbable ceramics in bone-tissue engineering and as coatings on metal implants to increase bioactivity. The first two compositions are frequently used in load-bearing implants. Additionally, various types of carbon are used as coatings or dialysis chambers in devices like heart valves. Additionally, a wide range of polymers is utilized as biomaterials. The flexibility, rigidity, strength, and bioinertness of polymers can range from low to high. To create a range of architectures, synthetic polymers can be functionalized with various biomolecules and treated using various techniques. Polymers are employed in various products, including prosthetic joints, skin, sutures, face implants, and medication delivery systems. The process of choosing materials for various biomedical devices is complex and is influenced by various elements, such as mechanical loading requirements, chemical and structural capabilities, and biological characteristics. Drug delivery and tissue engineering both involve biomaterials. Using nanostructures, various biomolecules and medications can be delivered to the target organ and subsequently regulated. Additionally, engineering biomaterials can result in multifunctional systems. Multipurpose biomaterials include magnetic nanoparticles.

Different medications can be loaded onto magnetic nanoparticles using an external magnetic field and delivered to a particular organ. In computed tomography and magnetic resonance imaging studies, some of these particles can also be employed to improve the contrast in the images. Another paradigm change has occurred in modern materials. Materials are carefully crafted to meet a variety of physiological parameters, but they also expand into the area of bioactive reactions. In other words, these materials go beyond the conventional definition of biocompatible by including elements that cause a beneficial biological interaction. The topics covered in these materials include biofouling, regenerative medicine, controlled release of pharmaceuticals, and tissue/organ engineering. Since the initial steel plates used for fracture fixation, these materials have come a long way, but there are still numerous obstacles to be overcome. Each application should satisfy biological criteria, and materials should be characterized. We are only beginning to comprehend the intricate processes and interactions between synthetic materials and our bodies because human biology is so complex. Various biomaterial kinds' general applications are shown in Fig. 1.3.

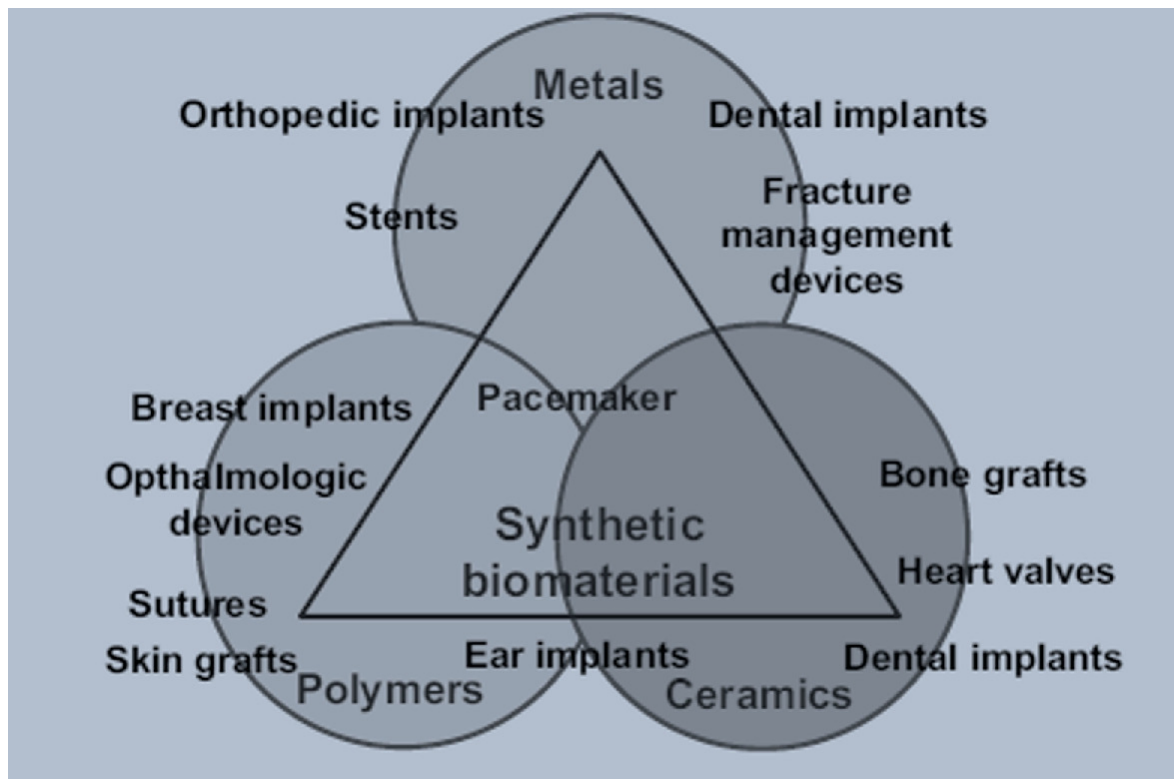


Fig. 1.3 Biomaterials application in different devices

1.6 Biomaterials Characterization

It is abundantly obvious from the previous discussion that the study of biomaterials is intrinsically multidisciplinary. When working on biomaterials to improve human health, researchers from the physical sciences, engineering sciences, biological sciences, and medicine frequently collaborate. Therefore, everyone must understand how to characterize different biomaterials and how to do so, which is the book's core focus. It's also critical to realize that, frequently, characterization of simply the biomaterials may not be sufficient, and additional systems-level testing may be required to confirm the device's actual functioning. This book was created to focus on the characterization of biomaterials and biomedical devices for their physical, mechanical, surface, in vitro, and in vivo biological properties, considering all those difficulties. Orthopedic and cardiovascular implants' device-level characterization received particular focus. Researchers in the physical and engineering disciplines have written chapters on biomaterials' physical, mechanical, and surface aspects. These chapters concentrate on methods for revealing fundamental features, including atomic structures, bonds, chemical interactions, phase identification, transformation, measures of strength and toughness, and an understanding of surface alterations and their impact on material properties. Biomaterials researchers use most of these strategies while developing new materials for specific uses.

1.7 Summary

This introductory chapter reviews materials, biomaterials, and the necessity to comprehend various methodologies to define biomaterials. The reader can understand how the other chapters' other topics are organized from this chapter to understand this fundamentally interdisciplinary discipline properly. Applying suitable characterization technologies can shorten the time needed to assess various biomaterials thoroughly and increase the safety of commercial biomedical devices. Safer biomedical technology will ultimately lessen human suffering, a goal all biomedical researchers share.

2. Atomic Structure

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

2.1 Explain Fundamental Concept of Atomic Structure (Theraja, 2000) From Modern Physics Aspects¹

Rutherford's Nuclear Atomic Model: It is considered that the massive positive portion of an atom is confined in an extremely small quantity at its center. The nuclei, the center of the atom, are encircled by an electron cloud, which makes the entire structure electrical neutrality.

Deficiencies in Rutherford's Nuclear Model:

1. Electron scattering outside of the nucleus.
2. The overall stability of the atom.

Bohr's Atomic Model

1. The nuclei of the atom are enormous and positively charged.
2. The electric attraction between the nucleus and the electrons balances the centrifugal force as the electrons move in a circular orbit around their nuclei.
3. An electron can only move in a limited number of distinct and definite orbits around its nucleus. These orbits are frequently referred to as stationary or stable orbits.
4. An electron emits no electromagnetic energy when rotating in these stable orbits.
5. Only when an electron moves from one orbit to another does the atom emit energy.

$$\Delta E = E_2 - E_1 = hf$$

$$E_2 = \text{Energy of orbit before jump}$$

$$E_1 = \text{Energy of orbit after jump}$$

$$h = \text{Plank's constant}$$

$$f = \text{Frequency of emitted photon}$$

Calculation Concerning Bohr's Atomic Model

(a) Radii of orbits:

$$R_n = \frac{\epsilon_0 n^2 h^2}{\pi m Z e^2} \quad (2.1)$$

which $n = 1, 2, 3, \dots$ orbit no.

Z Atomic no.

e charge = $1.6 \times 10^{-19} \text{C}$

ϵ_0 $8.854 \times 10^{-12} \text{F/m}$

h plank const. = $6.625 \times 10^{-34} \text{J.s}$

m mass of electron = $9.11 \times 10^{-31} \text{gm}$

(b) The velocity of Revolving Electrons:

$$v = 9 \times 10^9 \frac{2\pi Z e^2}{nh}$$

(c) Orbital Frequency:

$$f = \frac{m Z^2 e^4}{4 \epsilon_0^2 n^3 h^3}$$

(d) Electron Energy:

$$E_n = -\frac{m Z^2 e^4}{8 \epsilon_0^2 n^2 h^2}$$

Normal, Excited and Ionized Atom

One of our most basic atoms, H_2 , is thought to be in a normal (or unexcited) state when its lone electron is in its innermost orbit ($n = 1$). Throughout most cases, this is the state in which hydrogen atoms in a gas are produced to stay at standard room pressure and temperature. The atom is said to be ionized when the electron is eliminated from the atom. The atom is said to be excited if the electron is compelled into an outer or higher n -value orbit (or in an excited state). Because the electron moves to the lower expected orbit due to the nucleus' force of attraction, the atom does not stay in the excited state for more than 10^{-8} s.

Orbit of Shell

The nuclei have a positive charge numerically close to the atomic number (Z), which means no. of the proton, which determines the number of planetary electrons an atom can have. According to Bohr's model, each atom comprises positively charged nuclei with a certain quantity of electrons revolving around it in discrete or definite orbits. Bohr's orbits to which electrons are confined are called electron shells.

A shell is said to be filled or complete when it contains $2n^2$ electrons, where n is the shell or orbit number or principal quantum number.

Principal Quantum No. $\rightarrow$	$n = 1$	$n = 2$	$n = 3$	$n = 4$
Number of electrons $\rightarrow$	2	8	18	32

However, the maximum number of electrons a shell of any n -value can have is 32. It may be noted that

Orbit $n = 1 \rightarrow$ K-Shell

Orbit $n = 2 \rightarrow$ L-Shell

Orbit $n = 3 \rightarrow$ M-Shell

Electron Energy Level in Hydrogen Atom

The orbital energy of an electron revolving in the n th orbit of the shell is:

$$E_n = -\frac{mZ^2e^4}{8\epsilon_0^2n^2h^2}.$$

In the case of the hydrogen atom, $Z = 1$

$$E_n = -\frac{21.7 \times 10^{-19}}{n^2} \text{Joules}$$

But $1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$

$$E_n = -\frac{13.6}{n^2} \text{eV} \quad (2.5)$$

$\therefore$ For K-shell, $n = 1$; $E_1 = -13.6 \text{eV}$

$\therefore$ For L-shell, $n = 2$; $E_2 = -\frac{13.6}{2^2} = -3.4 \text{eV}$

$\therefore$ For M-shell, $n = 3$; $E_3 = \frac{-13.6}{3^2} = -1.51 \text{eV}$

ELD

It is common practice to sketch black lines to an energy peak rather than drawing different electron orbits to the peak of their radii. An atom's Energy Level Diagram (ELD) is one such diagram, as shown in Fig. 2.1. In this arrangement of energies, the greater (i.e., negative) energies are at the top, and the lesser energies are at the bottom.

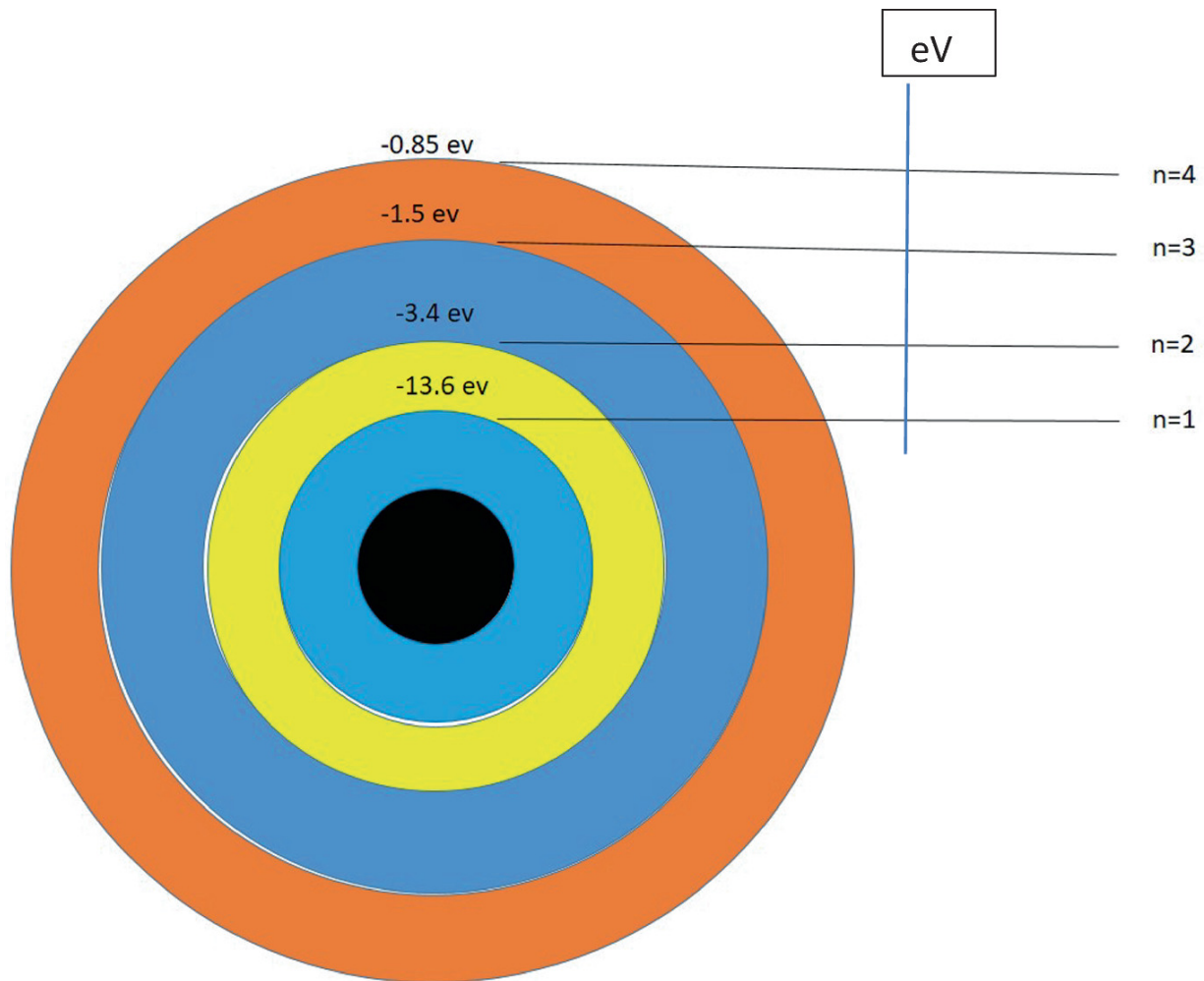


Fig. 2.1 Bohr's model applied to hydrogen spectra (Theraja, 2000)

In a normal unexcited hydrogen atom, the electron is still very much in the lowest level of energy at the bottom, i.e., in the innermost orbit with $n = 1$ (k-shell). It is also called the ground-state. The electron is stable in the ground state and revolves without emitting or absorbing any energy. The atom becomes excited when the electron absorbs energy by.

1. An accelerated particle heat the electron
2. Hydrogen may be heated so that the electron absorbs thermal energy
3. Hydrogen may be illuminated so that electron absorbs energy from photons.

In each of those cases, due to the absorption of energy, the electron is raised to one of the higher energy levels corresponding to the different values of n .

Ionization Energy

Suppose the electron of a hydrogen atom absorbs 13.6 eV. Then it is raised to $n = \infty$ level, i.e., the electron leaves the atom and drifts freely with only its thermal kinetic energy. The atom is considered to be ionized when the electron has been removed completely from it. The hydrogen atom's ionization energy is 13.6 eV in energy.

Excitation Energy

Suppose the electron of hydrogen absorbs the energy of 10.2 eV. In this case, it will be raised or excited from its lower level ($n = 1$) to the next higher permitted level ($n = 2$). It is so because the energy difference between those two states is $(13.6 - 3.4) = 10.2$ eV. This energy is called Excitation energy. Similarly, for being excited from $n = 1$ state to $n = 4$ state, the electron must absorb energy $= (13.6 - 0.85) = 12.75$ eV. The electron comes back to its lowest energy in about 10^{-8} s after excitation.

Special Series of Hydrogen Atom

The energy the hydrogen atom initially absorbed is released when it is excited, allowing it to come back to its lower energy level or ground state. The raised electron releases this energy as it transitions from a higher to a lower orbit via radiations with various wavelengths. This unique wavelength contributes to spectral series, one characteristic of the atom emitting them. These radiations are imaged as a single column's sharp, straight vertical lines when absorbed through a spectroscope. The frequency of the omitted radiations can be formed from the following relation:

$$hf = E_{n_2} - E_{n_1}$$

$$\text{where } E_{n_2} = -\frac{mZ^2e^4}{8\epsilon_0^2n_2^2h^2} = -\frac{me^4}{8\epsilon_0^2h^2} \cdot \frac{1}{n_2^2} [\text{H, } Z = 1]$$

$$E_{n1} = -\frac{me^4}{8 \epsilon_0^2 h^2} \cdot \frac{1}{n_1^2}$$

$$hf = \frac{me^4}{8 \epsilon_0^2 h^2} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$f = \frac{me^4}{8 \epsilon_0^2 h^3} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

But $c = f\lambda$ [c = velocity of light]

$$f = \frac{c}{\lambda}$$

$$\frac{c}{\lambda} = \frac{me^4}{8 \epsilon_0^2 h^3} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Let,

$$R = -\frac{me^4}{8 \epsilon_0^2 h^3 c} = 10.97 \times 10^6 m^{-1}$$

$$= \text{Rydberg's constant}$$

$$\therefore \frac{1}{\lambda} = R \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Now, wave number (σ) is given by the reciprocal of wave length, i.e.,
 $\sigma = \frac{1}{\lambda}$

$$\sigma = R \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad [\text{for hydrogen}] \quad (2.6)$$

This is the general expansion for the wave number of radiation emitted by an electron as it jumps from a higher energy level n_2 to a lower energy level n_1 .

Lyman Series

It is made up of all the wavelengths that an electron emits as it descends from a higher orbit to the $n = 1$ final orbit. In other words, all those electronic jumps which end at k-shell give Lyman series.

Here, $n_1 = 1, n_2 = 2, 3, 4, \dots, \infty$

$$\therefore \sigma = \frac{1}{\lambda} = R \left(\frac{1}{1^2} - \frac{1}{n_2^2} \right) = R \left(1 - \frac{1}{n_2^2} \right)$$

(a) First number ($n_2 = 2$)

$$\begin{aligned} \frac{1}{\lambda} &= R \left(1 - \frac{1}{2^2} \right) = \frac{3R}{4} \\ \therefore \lambda &= \frac{4}{3R} = \frac{4}{3 \times 10.97 \times 10^6} \\ \rightarrow \lambda &= 1216 \times 10^{-10} m \\ \lambda &= 1216 \text{Å} \end{aligned}$$

(b) 2nd number ($n_2 = 3$)

$$\lambda = \frac{9}{8R} = 1026 \text{Å}$$

(c) Limiting number ($n_2 = \infty$)

The limiting number of the series, i.e., the shortest wavelength of this series, is given by putting $n_2 = \infty$

$$\begin{aligned} \therefore \frac{1}{\lambda} &= R \left(1 - \frac{1}{\infty^2} \right) = R \\ \therefore \lambda &= \frac{1}{R} = \frac{1}{10.97 \times 10^6} \\ \therefore \lambda &= 91.2 \text{Å} \end{aligned}$$

This series of wavelengths lie in the ultraviolet region of the spectrum.

$$\therefore \text{Lyman series} : 91.2 \rightarrow 1216 \text{Å range}$$

Balmer Series

It comprises all the wavelengths released when various electron jumps end in an orbit with $n_1 = 2$.

$$\therefore \sigma = \frac{1}{\lambda} = R \left(\frac{1}{2^2} - \frac{1}{n_2^2} \right)$$

$$\therefore \frac{1}{\lambda} = R \left(\frac{1}{4} - \frac{1}{n_2^2} \right)$$

(a) 1st number ($n_2 = 3$)

$$\frac{1}{\lambda} = R \left(\frac{1}{4} - \frac{1}{3^2} \right) = \frac{5R}{36}$$

$$\therefore \lambda = \frac{36}{5 \times 10.97 \times 10^6} = 6563 \text{Å}$$

(b) 2nd number ($n_2 = 4$)

$$\lambda = \frac{16}{3R} = 4861 \text{Å}$$

(c) Limiting number ($n_2 = \infty$)

$$\lambda = \frac{4}{R} = 3646 \text{Å}$$

This series lies in the visible and near the ultraviolet regions of the solar spectrum.

$$\therefore \text{Balmer series Range} : 3646 \rightarrow 6563 \text{Å}$$

Paschen Series

It consists of all those wavelengths emitted when different electronic jumps end at $n_1 = 3$.

$$\therefore \frac{1}{\lambda} = R \left(\frac{1}{9} - \frac{1}{n_2^2} \right)$$

Brackett Series

When electronic jumps end at the orbit with $n_1 = 4$.

$$\therefore \frac{1}{\lambda} = R \left(\frac{1}{16} - \frac{1}{n_2^2} \right)$$

Pfund Series

When electronic jumps end at the orbit with $n_1 = 5$.

$$\therefore \frac{1}{\lambda} = R \left(\frac{1}{25} - \frac{1}{n_2^2} \right)$$

The last three series lie in the infra-red region of the spectrum.

Deficiencies in Bohr's Theory

1. While scientific data regarding the fine structure of spectral lines recommended different quantum numbers, the planetary model only wants to introduce one quantum number, n .
2. It only appears to apply to atoms with one electron, and it is difficult to extend it to describe more complex or multi-electron atoms.
3. No calculations regarding level transitions, such as their frequency or the selection criteria that apply to them, can be made using it.
4. It cannot be used for the quantitative explanation of chemical bonding. Thus, according to this theory, the calculation of bond strength (Bond-breaking energy) in the simplest system, like an ionized hydrogen molecule, gives a negative value suggesting that such an ion cannot exist. It does exist, and bond strength, in this case, is + 61 kcal/mole.

Sommerfeld's Relativistic Model

By continuing to expand Bohr's hypothesis in two ways, Sommerfeld partially managed to succeed in broadening the field of fine structure

1. In addition to Bohr's circular orbits, he enabled the possibility of elliptical orbits for the electrons.

2. He noted how the electron mass varied relativistically with velocity, differing at various points along the orbital motion.

When elliptical orbits are allowed, there are two variables that must be taken into account. These are in polar coordinates:

- (a) The distance between electron and nucleus, i.e., R .
- (b) The electron's transforming angular position with respect to the nucleus, i.e., the azimuthal angle ϕ .

To deal with these two variables, we need two quantum numbers:

1. In Bohr's theory, the original quantum number or principal quantum number n has been kept and is associated with the average distance between the electron and the nucleus. It also determines the energy of the electrons.

The orbital (or azimuthal) quantum number (l), another new quantum number, was once developed to characterize the angular momentum of an orbit, i.e., to evaluate the orbital angular momentum of the electron. In steps of unity, its value ranges from zero to $(n - 1)$. Finding potential elliptical orbits is made easier by using this orbital quantum number. Ellipse alternatives include:

$$\frac{b}{a} = \frac{l + 1}{n} \quad (2.7)$$

a and b are the ellipse's semi-major and semi-minor axes.

According to Sommerfeld's hypothesis, there are n possible sub-orbits or sub-shells of differing eccentricities for any given principal quantum number, n . These potential sub-orbits have different energies, which increases the relativistic variability of the electron mass (an electron's velocity tends to vary in an elliptical orbit but remains constant in a circular one). As a result, the velocity increases when the electron is close to the nucleus and decreases when it is farther away. Table 2.1 demonstrates that the optimum number of electrons permitted in any sub-shell is $= 2(l + 1)$, which is consistent with the special theory of relativity's prediction that the mass of the electron varies in the elliptical orbit.

Table 2.1 Electron Configuration where the maximum number of electrons allowed in any sub-shell is $= 2(2l + 1)$ (Theraja, 2000)

Sub-shell	K	L	M	N
Principal quantum number, n	1	2	3	4
Orbital number, l	0	/ \	/ \	/ / \ \
Possible electrons	1s	2s 2p	3s 3p 3d	4s 4p 4d 4f
Maximum number of electrons $2(2l + 1)$	2	2 6	2 6 10	2 6 10 14
Total number of electron $2n^2$	2	8	18	32

For $n = 1$, only one sub-shell is possible, having $l = 0$. For $n = 2$, two sub-shells are possible, having values of 0 and 1. For $n = 3$, three sub-shells are possible with $l = 0, 1, 2$. In other words, $0 \ll l \ll (n - 1)$ (Fig. 2.2).

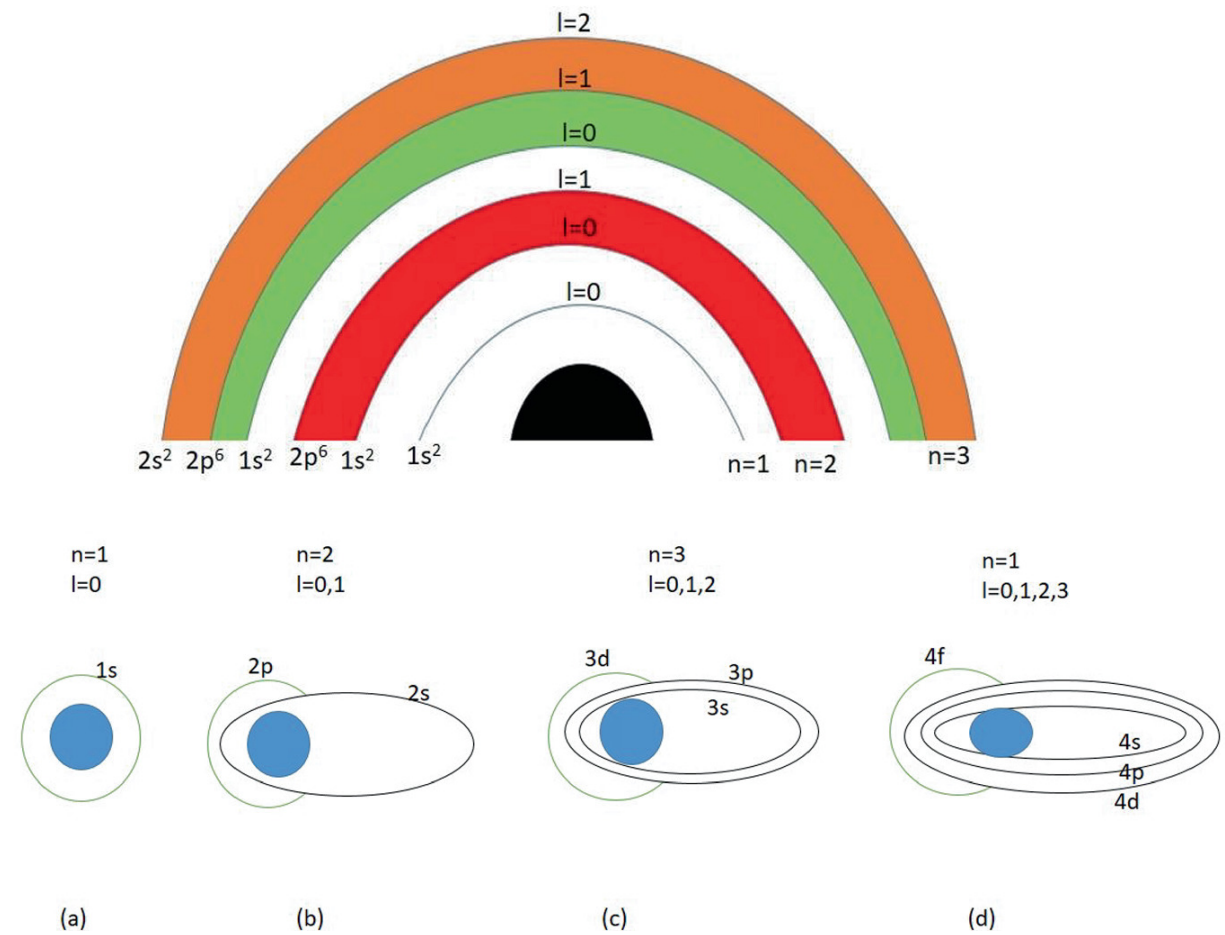


Fig. 2.2 Sommerfeld's relativistic model (Theraja, 2000)

For example, for $n = 4$, four sub-shells are possible.

$$(i) \ n = 4, l = 0$$

$$(ii) \ n = 4, l = 1$$

$$(iii) \ n = 4, l = 2$$

$$(iv) \ n = 4, l = 3$$

For

$$l = 3, \frac{b}{a} = \frac{3+1}{4} = 1;$$

Hence, $n = 4$, “” subs shell is circular as shown.

It is common practice to assign letters to $l - values$ as given below:

Orbital quantum, :	0	1	2	3	4	5
	↓	↓	↓	↓	↓	↓
Electron designation :	S	P	d	f	g	h

2.2 Explain Various Aspects of Electron Configuration of Atoms (Theraja, 2000) From Quantum Mechanics Point of View²

Following rules governing the electronic distribution:

- (a) The total number of electrons with the same principal quantum number (n) is $2n^2$.
- (b) In the n th shell, there are n -subshells having different values of orbital Q.N. (n), such as 0, 1, 2, ...($n-1$)
- (c) Each subshell can have a maximum of $2(2l + 1)$ electrons.

Aufbau Principle

According to this principle, electrons fill orbitals starting from the lowest available energy levels before filling higher, which means that orbitals with

lower $(n + l)$ values are filled before with higher $(n + l)$ values. i.e., 4s will be earlier than 3d.

Spin Quantum Number

To explain the doublets or double-line structure in the spectra of alkali metals, Goudsmit and Uhlenbeck postulated in 1925 that an electron spins around its axis as it moves in an orbit around the nucleus. For this purpose, they introduced another quantum number called electron spin quantum number, whose only possible value is $\frac{1}{2}$. The spin angular momentum is given by

$$P_s = s \cdot \frac{h}{2\lambda} \text{ when } s = \frac{1}{2}$$

Strictly speaking,

$$P_s = s \frac{h}{2\lambda}$$

where

$$s = [s(s + 1)]^{\frac{1}{2}}$$

Four Quantum Number

If we neglect the spin-orbit interaction, the following 4 quantum numbers can completely specify the state of an electron in an atom.

- (i) Principal Quantum Number (n)
- (ii) Orbital Quantum Number (l)
- (iii) Orbital Magnetic Quantum Number (m_l)
- (iv) Magnetic Spin Quantum Number (m_s).

The four quantum numbers express:

1. The principal quantum number (n) gives the position of an electron in the shell.
2. The orbital quantum number (l) gives the position of an electron in the sub-shell.
3. The orbital magnetic quantum number (m_l) gives its position in the sub-subshell.
4. The magnetic spin quantum number (m_s) gives the direction of spin or self-rotation, I.e., clockwise or anti-clockwise.

Orbital Magnetic Quantum Number (m_l)

This number arises because an electron in orbit contributes a rotating charge; an electric current has its associated magnetic field and magnetic moment. It is related to the orientation of elliptical electron orbits in space when the atom is placed in a magnetic field. These are restrictions on the orientation of the electron orbits because they are said to be space quantized. Whereas l determines the orbital angular momentum, m_l Represents the Z component of the orbital angular momentum. This Z direction is taken along the path of the applied field. The relationship between l and m_l Vectors are shown in the figure. Permitted values of θ are those for which $m_l = l \cos \theta$ It is an integer. It means that m_l Can have any of the $(2l + 1)$ values ranging from $-l$ to $+l$, including zero. i.e., $l, (l - 1), (l - 2) \dots 1, 0, -1, -2, \dots - (l - 2), - (l - 1) - l$. These values correspond to various sub-subshells in which electrons rotate around the nucleus (Fig. 2.3).

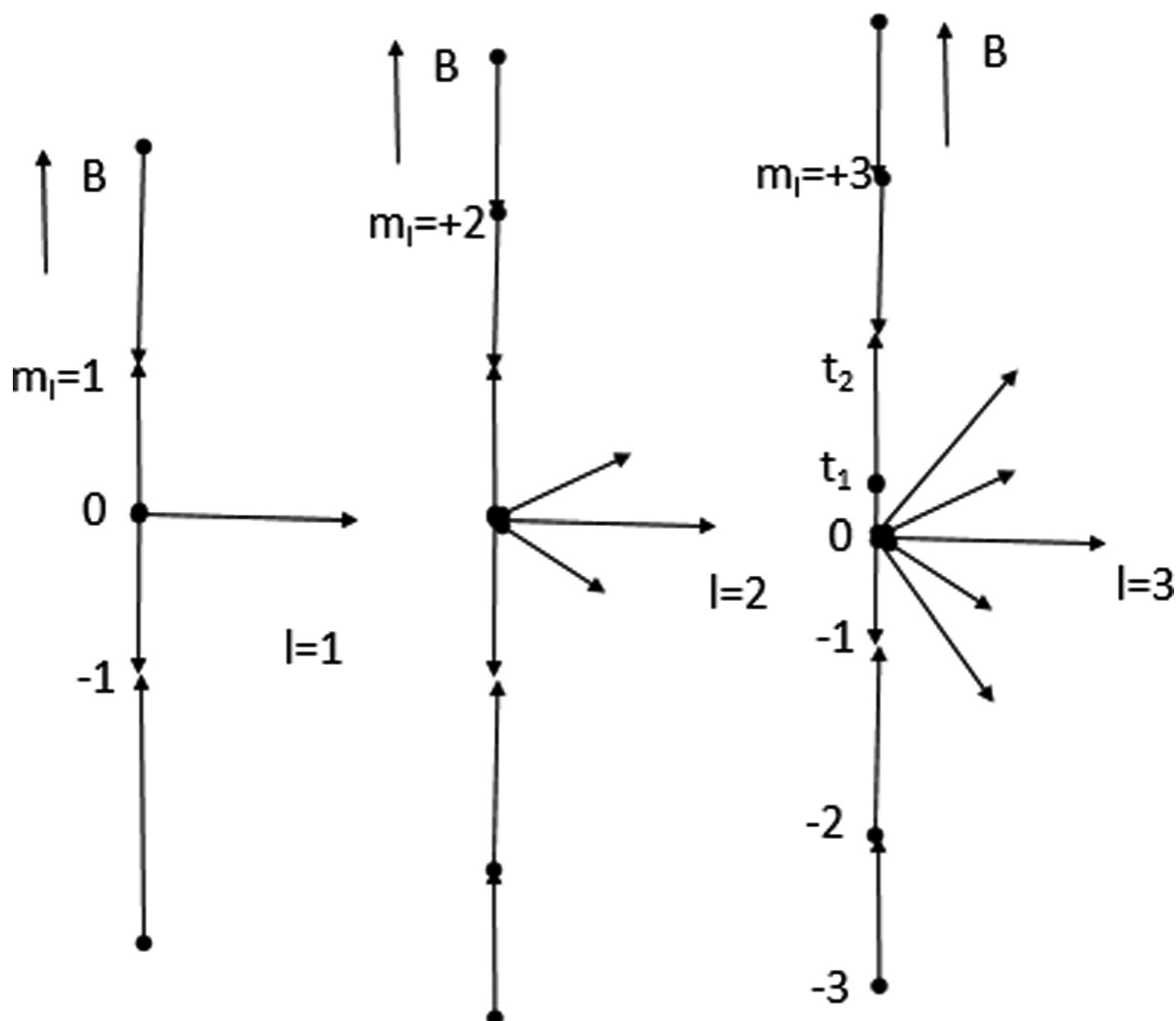


Fig. 2.3 Orbital magnetic quantum number (Theraja, 2000)

Magnetic Spin Quantum Number

It is the numerical value of the spin vector “s” projection on the field direction. This spin vector can only be oriented in either of the two ways: parallel or anti-parallel to the surrounding magnetic field. Hence, m_s can have only two values; $+\frac{1}{2}$ or $-\frac{1}{2}$ which differ by unity, as do all other quantum numbers.

Pauli’s Principle

It states that in one atom, no two electrons can have the same set of values for the four quantum numbers n , l , m_l and m_s . They may have three

numbers, but at least one must be different. Considering the case of Helium which has two electrons in its atom. These electrons occupy the k-shell ($n = 1$) and are designated $1s^2$ electrons. These four quantum numbers are:

	N	l	m _l	m _s
1st electron :	1	0	0	$+\frac{1}{2}$
2nd electron :	1	0	0	$-\frac{1}{2}$

As seen, the two electrons have different sets of four numbers ($1, 0, 0, +\frac{1}{2}$) and ($1, 0, 0, -\frac{1}{2}$) as required by Pauli's Principle.

The hydrogen atom does not demonstrate this rule for the simple reason that it has one electron only.

Significance of Quantum Number

(a) Principal Quantum Number

First is the Principal Quantum Number (n), which varies from unity to infinity in steps of unity. It consists of electron energy and determines the electron orbit's size.

(b) Orbital Quantum Number

The second is the Orbital Quantum Number (l), which takes integral values ranging from 0 to $(n-1)$ in steps of unity. It determines the electron's angular momentum about the nucleus and the shape or eccentricities of the electron orbits.

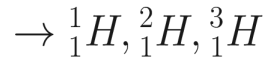
(c) Orbital Magnetic Quantum Number (m_l)

The third is Orbital Magnetic Quantum Number (m_l), which takes integral values from $(-l)$ to $(+l)$ in steps of unity. It defines the angular momentum parallel to an applied magnetic field. It determines the orientation (position) of the electron orbit in space.

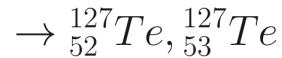
(d) Magnetic Spin Quantum Number (m_s)

Fourth is Magnetic Spin Quantum Number (m_s), which takes values of $+\frac{1}{2}$, the sign depending on whether it is parallel or anti-parallel to the orbital magnetic quantum number (m_l). It determines the spin orientation up or down.

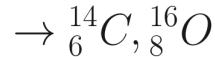
Isotope: mass different, same proton



IsoBar: mass same, proton different



Isotone: mass and proton different, neutron same



Atomic Mass (A) : P + N (Proton + Neutron)

Atomic Number (Z) = P = Proton Number
= Electron number

Footnotes

1 Chapter 2 to 7 are written including compiled data for tables and redrawn schematics based on the references B. L. Theraja, 2000, "Modern Physics", S. Chand & Company Ltd. New Delhi, India, A. Pytel & F. L. Singer, 1995, "Strength of Materials", Haper & Row, New York, USA, J. P. Schaffer, A. Saxena, S. D. Antolovich, T. H. Sanders, and Steven B. Warner, 1999, "The Science and Design of Engineering Materials", WBC/McGraw-Hill, USA, Sydney H. Avner, 1997, "Introduction to Physical Metallurgy", Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, "Foundations of Materials Science and Engineering", 2004, McGraw-Hill, 3 Ed, New York, USA and William D. Callister Jr. & David G. Rethwisch, 2009, "Materials Science and Engineering: An Introduction", 8th ed. John Wiley and Sons. NJ, USA.

2 Chapter 2 to 7 are written including compiled data for tables and redrawn schematics based on the references B. L. Theraja, 2000, "Modern Physics", S. Chand & Company Ltd. New Delhi, India, A. Pytel & F. L. Singer, 1995, "Strength of Materials", Haper & Row, New York, USA, J. P. Schaffer, A. Saxena, S. D. Antolovich, T. H. Sanders, and Steven B. Warner, 1999, "The Science and Design of Engineering Materials", WBC/McGraw-Hill, USA, Sydney H. Avner, 1997, "Introduction to Physical Metallurgy", Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, "Foundations of Materials Science and Engineering", 2004, McGraw-Hill, 3 Ed, New York, USA and William D. Callister Jr. & David G. Rethwisch, 2009, "Materials Science and Engineering: An Introduction", 8th ed. John Wiley and Sons. NJ, USA.

3. Crystallography

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

3.1 Explain Fundamental Concept of Crystal Structure (Theraja, 2000 and Avner, 1997) From Materials Science Aspects¹

A crystal is a three-dimensional repetition array of atoms. This means that atoms are arranged in a periodically repeating geometric array.

Space Lattice

The 3-dimensional network of imaginary lines connecting the atoms is called a space lattice. Or the angular arrangement of the space positions of the atoms in a crystal is called space lattice or lattice array.

Unit Cell

The smallest unit with the crystal's full symmetry is called the unit cell. Or the smallest block or geometric figure from which the crystal is built up by repetition in three dimensions.

Lattice Parameters

The three sides of a unit cell are called the crystallographic axes. The angles between the three axes are called interfacial angles. The intercepts a , b and c define the dimensions of a unit cell and are known as its primitives or characteristic intercepts on the axes. The primitives and interfacial angles constitute the lattice parameters of the unit cell. These are also called the geometrical constants of given crystal substances (Fig. 3.1).

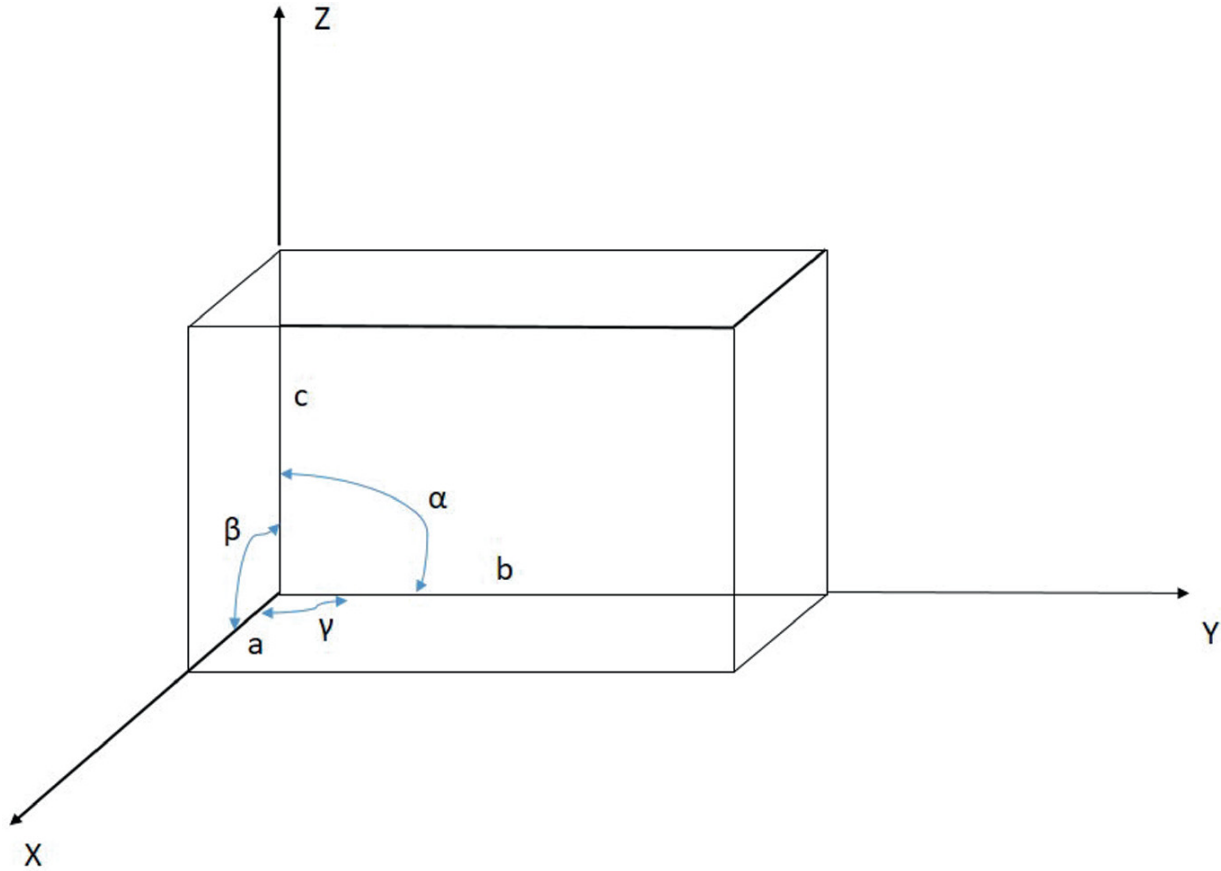


Fig. 3.1 Lattice parameter (Theraja, 2000)

In a space lattice, all lattice points may be included in a set of parallel and equally-spread planes known as lattice planes. These planes give the orientations of possible faces of a crystal of the substances. In theory, there are 320 such lattices divided into 32 crystal classes. These can be arranged in 7 crystal systems which are characterized by three symmetry elements: (i) the plane of symmetry, (ii) The axes of symmetry, and (iii) the center of symmetry.

The Seven Crystal System

There are seven crystal systems corresponding to seven distinct types of unit cells. These unit cells are all parallelepiped whose shapes are determined by primitives (a , b , and c) and the values of the interfacial angles (α , β , γ). These systems are 1. Cubic 2. Monoclinic 3. Triclinic 4. Tetragonal 5. Orthorhombic 6. Rhombohedral (Trigonal) 7. Hexagonal (Table 3.1).

Table 3.1 Crystal structure (the seven crystal system) (Theraja, 2000)

S. No.	Name of the system	Relation between primitives	Interfacial angles	Example
1	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	NaCl, CaF_2 , NaClO_2
2	Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$	Na_2SO_4 , FeSO_4
3	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	CuSO_4 , $\text{K}_2\text{Cr}_2\text{O}_7$
4	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	NaSO_4 , SnO_4
5	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	KNO_3 , BaSO_4 , MgSO_4
6	Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	CaSO_4
7	(Trigonal) Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	SiO_2 , AgI

Bravais' Lattice

Bravais introduced the space lattice idea as early as 1880. There are 14 possible space lattices in these seven crystal systems: 1 triclinic, 2 monoclinic, 4 orthorhombic, 2 tetragonal, 1 hexagonal, 1 rhombohedral and 3 cubics. It has been proved mathematically that there are only 14 independent ways of arranging points in 3D space such that each arrangement conforms to the definition of a space lattice.

Symmetry Elements of a Crystalline Solid

If $n = 1$, the crystal has to be rotated through 360° to achieve self-coincidence; this axis is called an Identity axis.

If $n = 2$, the crystal has to be rotated through 180° to achieve self-coincidence, and the axis is called a Diad axis.

If $n = 3$, the rotation angle is 120° and the Triad axis.

If $n = 4$, the rotation angle is 90° , and the Tetrad axis.

If $n = 6$, the rotation angle is 90° , and the axis is called Hexad, where “n” indicates the n-fold axis of symmetry. [complete revolution $360^\circ/n$].

It is found that crystalline solids show only 1, 2, 3, 4 and sixfold symmetry. They do not show fivefold or any symmetry axis higher than 6. There are 23 elements of symmetry.

1. 13 axes of symmetry—3 tetrads, 4 triads and 6 diads.
2. 9 planes of symmetry—3 planes parallel to the faces of the cube and 6 diagonal planes.
3. 1 centers of symmetry.

The unit cells belonging to the seven crystal systems have the following symmetry axes:

1. The triclinic system has no axis of symmetry.
2. The monoclinic system has one diad axis only. Moreover, there are no axes of higher degrees.
3. The orthorhombic system has 3 diad axes only.
4. The rhombohedral system has one fourfold axis. This unique axis is called the c-axis. (i.e., Z -axis).
5. The cubic system has 4 triad axes.
6. The tetragonal system has one triad axis. This unique axis is equally inclined to the three coordinate axes.
7. The hexagonal system has one hexad. This unique axis is at the right angle to the other coordinate axes.

Space Lattices of Cubic System

This system makes three types of space lattices possible depending on the positions of the lattice points in the unit cells.

1. Simple Cubic (SC) lattice
2. Body-Centred Cubic (BCC) lattice

3. Face-Centred Cubic (FCC) lattice.

Coordination Number

Coordination numbers are the number of nearest neighbours atom an atom has in the unit cell of any crystal structure.

1. Simple Cubic (SC) Lattice

In this case, the coordination number is 6. It is so because each corner atom is linked with seven other unit cells containing the atom. In that case, each corner atom has four neighbours in the same plane, one vertically and one immediately below, giving a total of 6 nearest neighbouring atoms (Fig. 3.2).

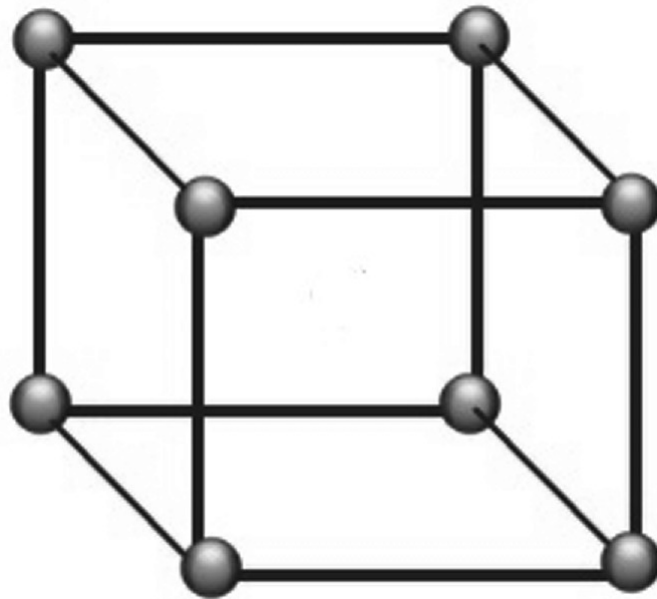


Fig. 3.2 SC (simple cubic) structure (Theraja, 2000)

2. Body-Centred Cubic (BCC) Structure

Its coordination number is 8. In this case, the nearest neighbours of any corner atom are the Body-Centred atom (and not the other corner atoms). Since there are 8 surrounding unit cells for any corner atom, their 8 body-centered atoms form the nearest neighbor for any corner

atom. If the atoms are represented as spheres, the center atom touches each corner atom, but these corner atoms do not touch each other. Since each corner atom is shared 8 adjoining unit cells and the atom in the center cannot be shared by any other unit cell, each unit cell of the BCC structure contains (Fig. 3.3):

$$\begin{aligned}
 8 \text{ atoms at the corner} \times \frac{1}{8} &= 1 \text{ atom} \\
 1 \text{ center atom} &= 1 \text{ atom} \\
 \text{Total} &= 2 \text{ atoms}
 \end{aligned}$$

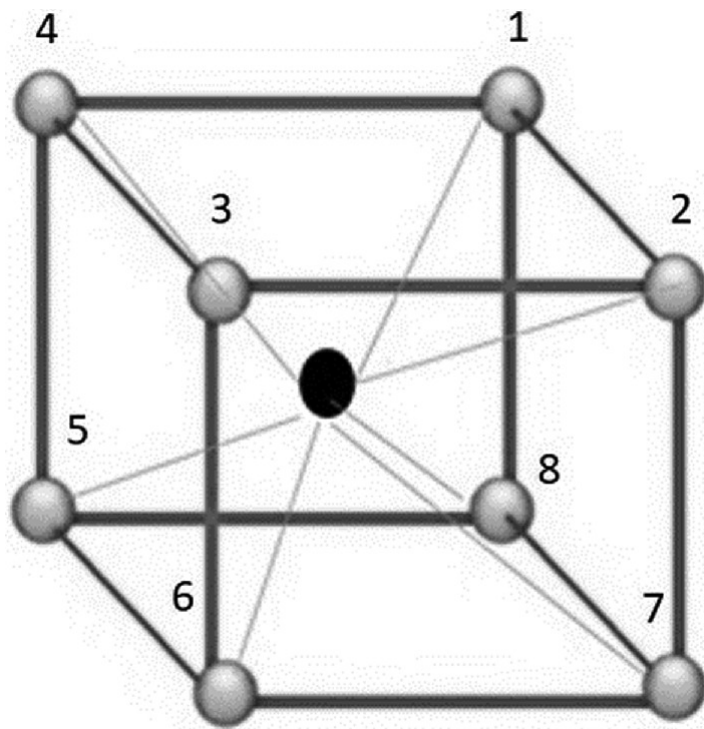


Fig. 3.3 BCC (body-centred cubic) structure (Theraja, 2000)

Example: BCC structures are Chromium, Tungsten, α -Iron, γ -Iron, Molybdenum, Vanadium, Sodium and Titanium.

3. Face-Centred Cubic (FCC) Structure

The coordination number of an FCC structure is 12. In this case, the nearest neighbors of any corner atoms are the face-centered atoms of the surrounding unit cells. Any corner atom has four such atoms in its place, four in a plane above it and four below it. In addition to an atom at each corner of the unit cell, there is one in the center of each face but

none in the center of the unit cell. Each face atom touches its nearest corner atom. Since each corner atom is shared by 8 adjoining unit cells and each face atom is shared by one adjacent unit cell, each unit cell contains (Fig. 3.4):

$$\begin{aligned}
 8 \text{ atoms at the corners} &\times \frac{1}{8} = 1 \text{ atom} \\
 6 \text{ face-centred atoms} &\times \frac{1}{2} = 3 \text{ atoms} \\
 \text{Total} &= 4 \text{ atoms}
 \end{aligned}$$

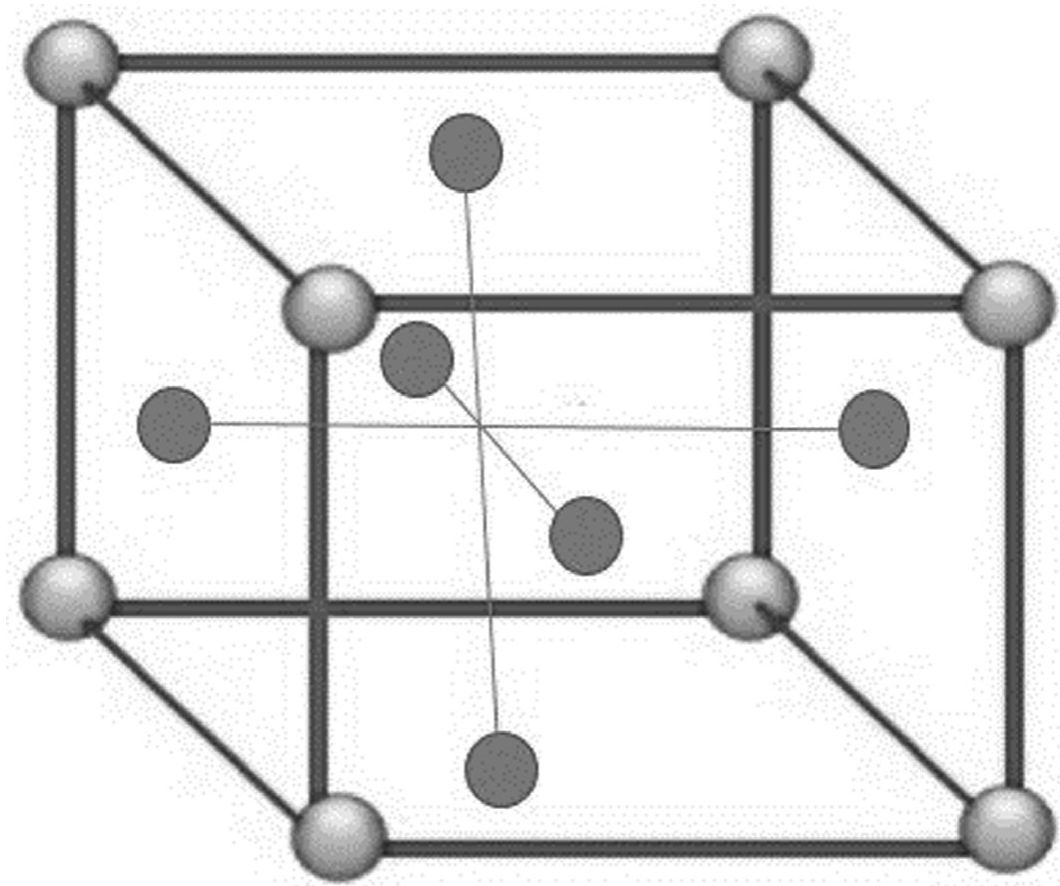


Fig. 3.4 FCC (face-centred cubic) structure (Theraja, 2000)

The FCC structure is more densely packed than the BCC structure.
Example: Al, Cu, Au, Pb, Ni, Platinum, Ag and γ -Iron.

Packing Factor

The fraction of the volume of a unit cell occupied by the volume of atoms.

In FCC, since there are 4 atoms per unit cell and each atom is a sphere of radius R_a , then, $V_{atoms} = 4 \left(\frac{4}{3} \pi r_a^3 \right) = \frac{16}{3} \pi r_a^3$ and $V_{cell} = a^3$ [a = primitives].

$$a\sqrt{2} = 4r_a$$

$$\rightarrow a = 2\sqrt{2}r_a$$

$$\therefore \text{Packing factor} = \frac{V_{atoms}}{V_{cell}} = \frac{\frac{16}{3} \pi r_a^3}{(2\sqrt{2}r_a)^3} = \frac{\pi}{3\sqrt{2}} = 0.74$$

FCC Packing Factor = 0.74 and BCC Packing Factor = 0.68 (Table 3.2).

Table 3.2 Summary of SC, BCC and FCC structure (Theraja, 2000)

	SC	BCC	FCC
Coordination number	6	8	12
Atomic radius (r_a)	$\frac{a}{2}$	$\frac{\sqrt{3}}{4} \cdot a$	$\frac{\sqrt{2}}{4} \cdot a$
Atoms per unit cell	1	2	4
Density of packing	$\frac{\pi}{6}$	$\frac{\sqrt{3}}{8} \pi$	$\frac{\sqrt{2}}{6} \cdot \pi$

Close Pack Hexagonal (CPH) Structure

The usual picture of the close-packed hexagonal lattice shows 2 basal planes in the form of regular hexagons with an atom at each corner of the hexagons and one atom at the center. In addition, there are 3 atoms in the structure of a triangle midway between the two basal planes. If the basal plane is divided into nine equilateral triangles, the additional three atoms are nestled in the center of alternate equilateral triangles. Since each atom at the corner of the unit cell is shared by eight adjoining cells and one atom inside the cell cannot be shared, the CPH unit cell contains two atoms. The unit cell of the hexagonal cell is specified by the width of the hexagon (a) and the distance between basal planes (c). These determine the axial ratio (c/a). The axial ratio of a CPH structure formed of spheres in contact is 1.633. In reality, metals of this structure have axial ratios that vary from 1.58 for Beryllium to 1.88 for Cadmium. Example: Mg, Be, Zn, Cd, Hg, C and Ti (Fig. 3.5).

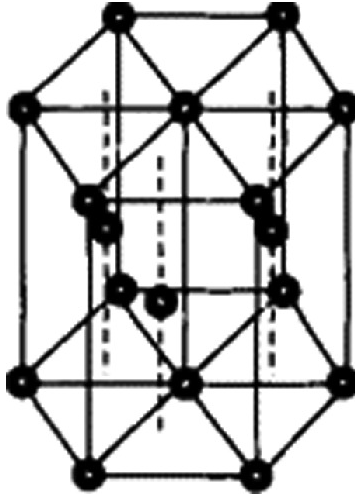


Fig. 3.5 HCP (hexagonal close-packed) structure (Theraja, 2000)

Polymorphism and Allotropy

Polymorphism is the property of a material to exist in more than one type of space lattice in the solid state. If the change in structure is reversible, then the polymorphic change is known as allotropy. At least 15 metals show this property; iron is the least-known example. When iron crystallizes at 2800 °F, it is BCC (γ -Fe); at 2544 °F, the structure changes to FCC (γ -Fe), and at 1670 °F, it again becomes (α -Fe).

Crystallographic Planes and Miller Index

The layers of atoms or the planes arranged by atoms are crystallographic planes. The relation of a set of planes to the axes of the unit cell is designated by Miller Indices. One corner of the unit cell is assumed to be the origin of the space coordinates. Any set of planes is identified by the reciprocals of its intersections with these coordinates. The unit cell of the coordinates is the lattice parameter of the crystal. If a plane is parallel to an axis, it intersects at infinity (Fig. 3.6).

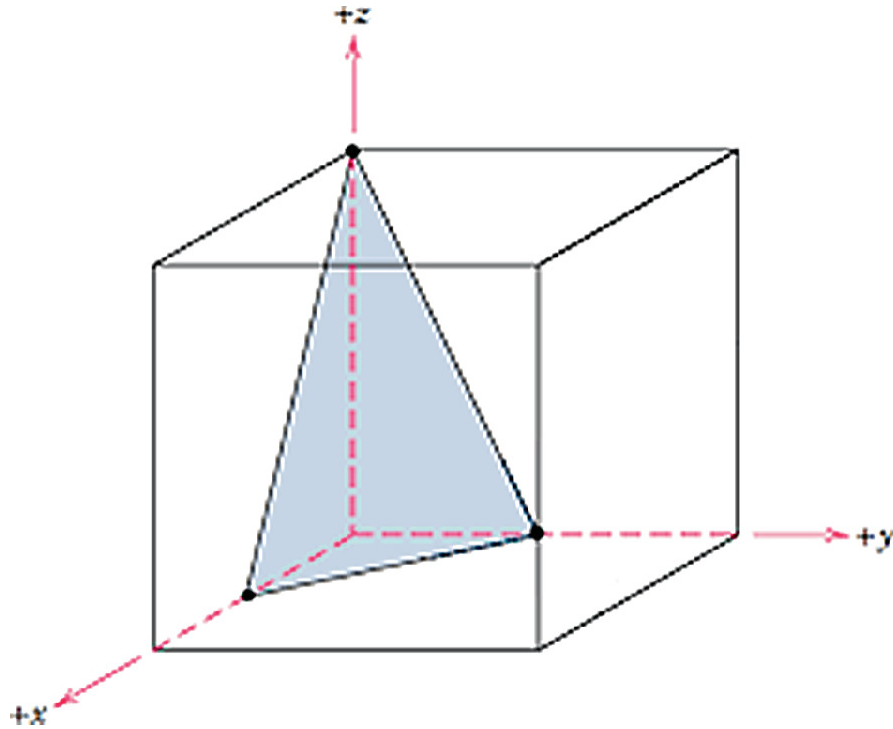


Fig. 3.6 Crystallographic planes (Theraja, 2000)

From the figure of the cubic system, the crosshatched plane BEHG intersects the y-axis at 1 unit from the origin and is parallel to the X and Z axes or intersects them at infinity. Therefore (Table 3.3).

Table 3.3 Miller index for BCHG plane (Avner, 1997)

	X	Y	Z
Intersection	∞	1	∞
Reciprocal	$\frac{1}{\infty}$	$\frac{1}{1}$	$\frac{1}{\infty}$
Miller index	0	1	0

∴ The BCHG plane has a Miller index of (010). If a plane cuts any axis on the negative side of the origin, the index will be negative and is indicated by placing a minus sign above the index as ($h\bar{k}l$). For example, the Miller Index of the plane ADEF, which goes through the origin (Point A), can't be determined without changing the location of the origin. Any point in the cube may be selected as the origin. For convenience, taking point B. The plane ADEF is parallel to the x-axis (BC) and the Z axis (BG) but intersects the Y-axis at -1. The plane has Miller indices of ($0\bar{1}0$). The Miller Index of the plane BDJ may be determined as follows (Table 3.4).

Table 3.4 Miller index for BDJ plane (Avner, 1997)

	X	Y	Z
Intersection	1	1	$\frac{1}{2}$
Reciprocal	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{\frac{1}{2}}$
Miller index	1	1	2

∴ BDJ Plane has a Miller Index of (112). If the Miller Index of the plane results in fractions, these fractions must be cleared. For example, considering a plane intersects at the x-axis at 1, y-axis at 3 and Z-axis at 1. Taking the reciprocals gives an index of 1, 1/3, and 1. Multiplying by 3 to clear fractions results in a Miller Index of (313) for that plane.

Important Plane System in a Cubic Crystal

There are 3 sets of planes rich in atoms in a cubic crystal. Consequently, Bragg's reflections from these planes are more intense than others. These three sets of planes are:

1. The 1st set of planes consists of surface planes of the cube and those parallel to them, such as BFGC, AEHD, ABCD, and EFGH. Let the distance between connective parallel surface planes be d_1 .
2. The 2nd set of planes consists of parallel planes like AFGD, which are inclined at an angle of 45° to the plane of 1st set. Let their spacing d_2 .
3. The 3rd set of planes consists of those planes parallel to the plane AFH. Let the spacing be d_3 (Fig. 3.7).

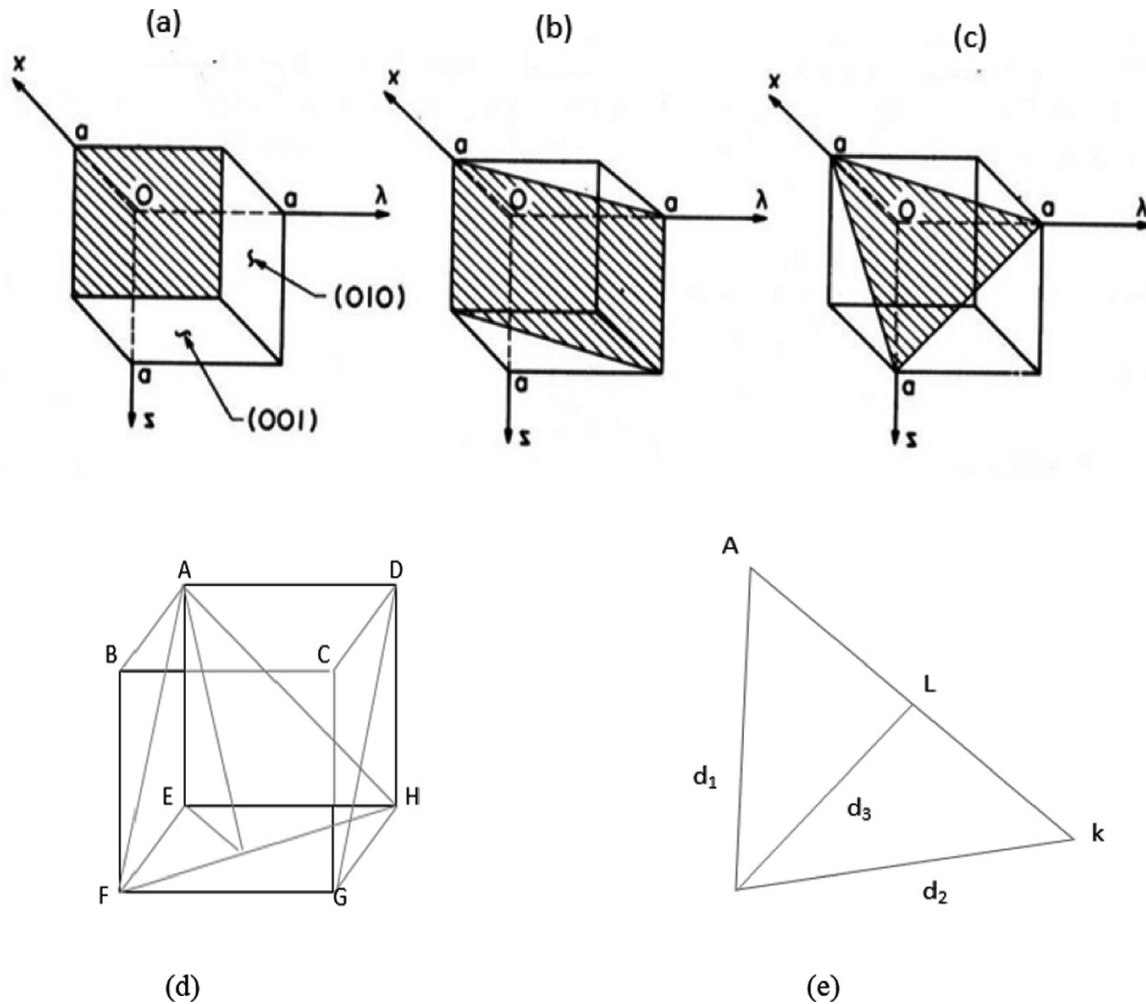


Fig. 3.7 Spacing of planes (Theraja, 2000)

Knowing the spacing of these sets of planes is essential for identifying different types of crystals. It is so because a definite ratio exists between the spacing of planes rich in atoms for each basic crystal structure.

We are considering the case of a simple cubic crystal with atoms at the cube's corners, as shown in (a). The spacing of face planes like ABCD and EFGH is d_1 .

The spacing of planes like AFGH, which are inclined at 45° to the 1st set of planes, is $d_2 = d_1/\sqrt{2}$.

The $\triangle AFH$ represents the 3rd set of planes whose spacing d_3 may be formed by drawing the $\triangle AEK$ in shape in figure ©.

In figure (d), $EK \perp FH$ and $EL = d_3 \perp AK$.

From two similar $\triangle ELK$ and $\triangle AEK$ from figure (d), we get,

$$\frac{EL}{EK} = \frac{AE}{AK}$$

$$\rightarrow \frac{d_3}{d_2} = \frac{d_1}{\sqrt{d_1^2 + d_2^2}}$$

$$d_3 = \frac{d_1 d_2}{\sqrt{(d_1^2 + d_2^2)}}$$

Now, putting $d_3 = d_1/\sqrt{2}$, we get

$$\therefore d_3 = \frac{d_1^2}{\sqrt{2}\sqrt{(d_1^2 + \frac{1}{2}d_1^2)}} = \frac{d_1}{\sqrt{3}}$$

$$\therefore \frac{1}{d_1} : \frac{1}{d_2} : \frac{1}{d_3} = 1 : \sqrt{2} : \sqrt{3} \quad [\text{simple cubic}]$$

Similarly, it can be shown that for a BCC: $\frac{1}{d_1} : \frac{1}{d_2} : \frac{1}{d_3} = 1 : \frac{1}{\sqrt{2}} : \sqrt{3}$ [BCC].

And for FCC:

$$\frac{1}{d_1} : \frac{1}{d_2} : \frac{1}{d_3} = 1 : \sqrt{2} : \frac{\sqrt{3}}{2} \quad [\text{FCC}]$$

From the reflection of monochromatic x-rays from different crystals and the above ratios, it can be determined whether SC, BCC or FCC can be determined.

3.2 Explain Various Aspects in Mechanism of Crystallization (Avner, 1997) From Materials Science Point of View²

Crystallization is the transition from the liquid to the solid state and occurs in two stages. 1. Nucleation 2. Crystal growth.

1. Nucleation

Although the atom in the liquid state does not have any definite arrangement, some atoms at any given instant may be in a position

exactly as the space lattice, which was assumed when solidified. These chance aggregates or groups of tiny particles are called Nuclei, and the formation of these chance aggregates is called nucleation. These chance aggregates or groups are permanent but continually break up and reform at other points. How long they last are determined by the group's temperature and size. The higher the temperature, the greater the kinetic energy of the atoms and the shorter the group's life. When the liquid temperature decreases, the atom movement decreases, and more groups will be present at that same time.

Atoms in a material have both kinetic and potential energy. Kinetic energy is related to the speed at which the atoms move and is strictly a function of temperature. The higher the temperature, the more active the atoms are and the greater their KE. Potential Energy (PE) is related to the distance between atoms. The greater the average distance between atoms, their potential energy is greater. The atoms in the liquid and the solid must be the same, but there is a significant difference in PE. The atoms in a solid are much closer together, so solidification occurs with a release of energy. This difference in PE between the liquid and solid states is known as the latent heat of fusion. Energy is required to establish a surface between the solid and liquid. In pure materials, insufficient is released by the latent heat of fusion to create a stable boundary at the freezing point. This is why some undercooling is always necessary to form stable nuclei. Subsequent release of the latent heat of fusion will raise the temperature to freeze. The amount of undercooling required can be reduced by solid impurities, reducing the surface energy required. When the liquid metal temperature has dropped sufficiently below its freezing point, stable aggregates or nuclei appear spontaneously at various points in the liquid (Fig. 3.8).

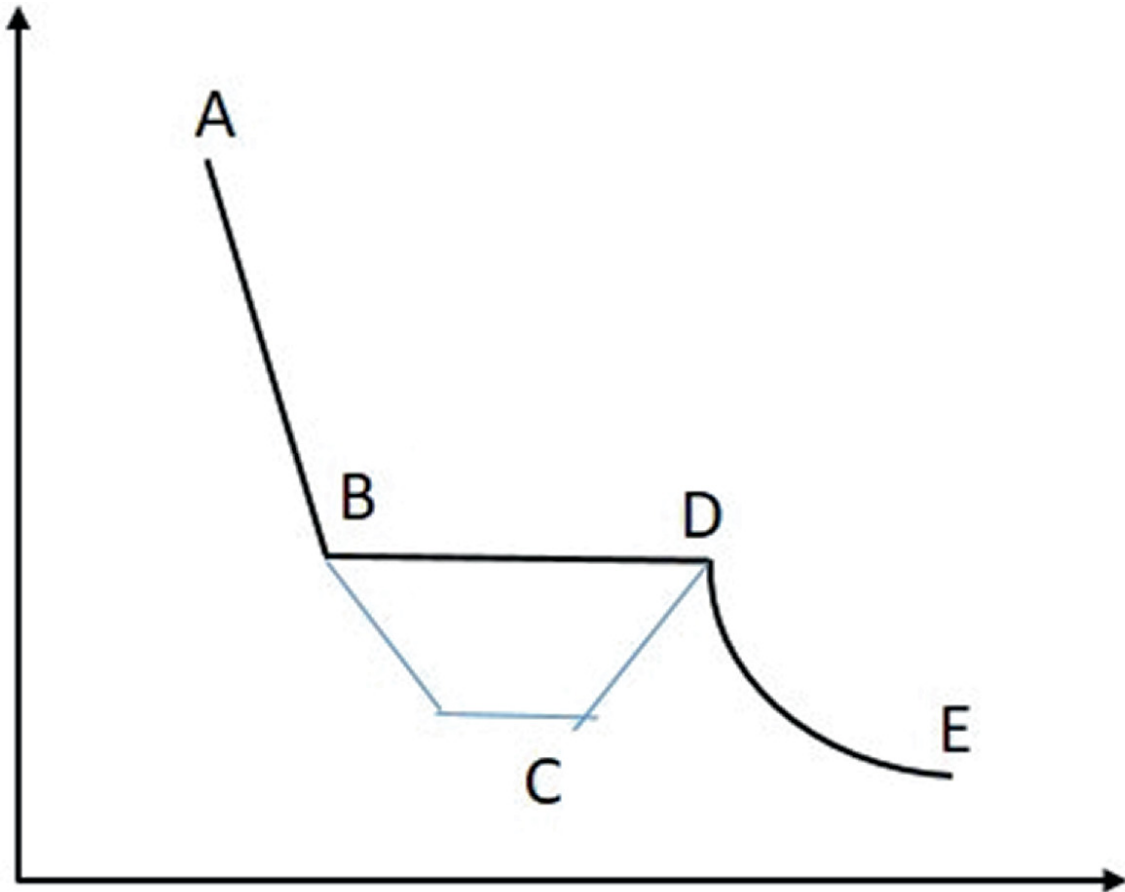


Fig. 3.8 Cooling curve for a pure metal (ABDE = Ideal & ABCDE = Real) (Avner, 1997)

The crystals formed in all commercial metals are commonly called a grain because of the variation in external shape.

2. **Crystal Growth or Grain Growth or Nucleation Growth**

Those nuclei, which have solidified, act as centers for further crystallization. As cooling continues, more atoms freeze and may attach themselves to existing nuclei or form new ones. Each nucleus grows by the attraction of atoms from the liquid into its space lattice. Crystal growth continues in 3-Dimensions, allowing attaching themselves in certain preferred directions, usually along the axes of the crystal. This gives rise to a characteristic tree-like structure which is called Dendrite. Since each nucleus is formed by chance, the crystal axes are pointed at random, and the dendrites growing from them will grow in different directions in each crystal. Finally, as the number of liquid decreases, the gaps between the arms of the dendrite will be filled, and that of its neighbours will mutually obstruct the growth of the dendrite. This leads to a very irregular external shape. The crystals formed in all

commercial metals are called grains because of this variation in external shape. The area where crystals meet is the Grain Boundary in a mismatch region. This leads to a non-crystalline or amorphous structure with the atoms irregularly spaced at the grain boundary. Since the last liquid to solidify is generally along the grain boundary, there tends to be a higher concentration of impurity atoms in that area.

3.3 Explain Various Aspects of Crystal Imperfections (Avner, 1997) From Materials Science Point of View³

The defects in the crystal structures are called Crystal Imperfections. They are 1. Vacancies 2. Interstitials 3. Dislocations—Edge Dislocations and Screw Dislocations.

Vacancies

Vacancies are simply empty atom sites. A vacancy can be formed by an atom migrating from a normal lattice site to the surface of the crystal. This is known as a Schottky Defect. The atoms surrounding a vacancy tend to be closer together, distorting the lattice planes. The formation of Schottky defects results in volume expansion and hence density decrease. The migration of an atom from a normal lattice site to an interstitial site can also form a vacancy. This is known as a Frankel Defect. Formation of Frankel Defects doesn't affect the density (Fig. 3.9).

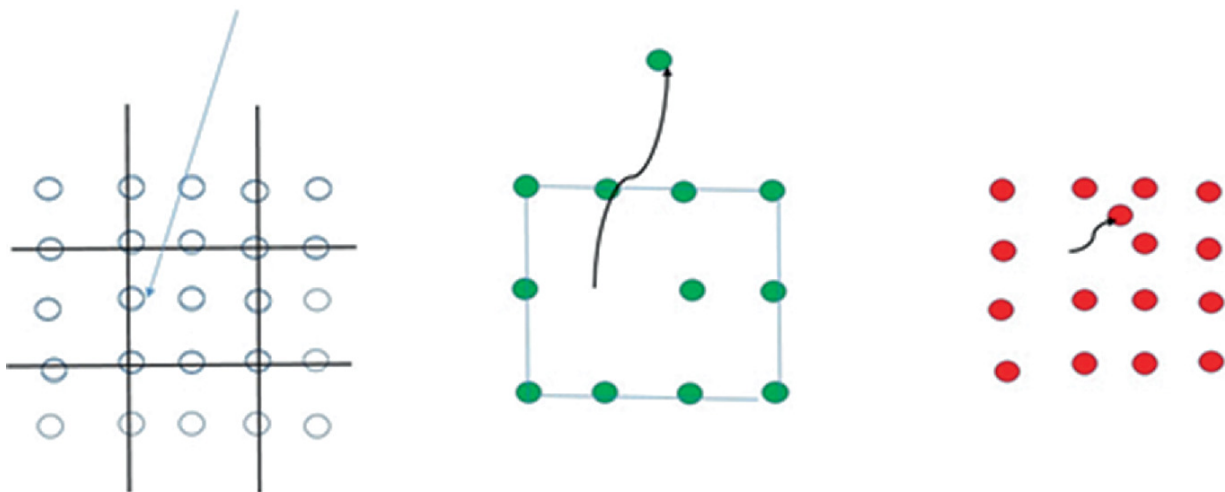


Fig. 3.9 Crystal imperfections (Vacancies) (Avner, 1997)

They are considering TiO_2 . When heated in a vacuum, oxygen denotes from the crystal, producing oxygen anion vacancies. The compound is now TiO_{2-x} ($x > 0$). If the oxygen loss is small, there is no major structural change. The two electrons associated with the oxygen anion remain but are no longer fixed in the oxygen site to maintain electrical neutrality. This affects the electrical and optical properties of TiO_2 . Pure TiO_2 is an insulator with a yellowish tint. After heating in a vacuum, TiO_2 turns blue and is electrically conducting.

Interstitials

It is possible, particularly in a lattice structure, that some atoms may fall into interstitial positions or in the spaces of the lattice structure. Interstitials tend to push the surrounding atoms further apart and distort the lattice planes. Vacancies are not only present as a result of solidification but can be produced by raising the temperature or irradiating with fast-moving nuclear particles. The severe local distortion produces interstitial atoms during plastic deformation and irradiation (Fig. 3.10).

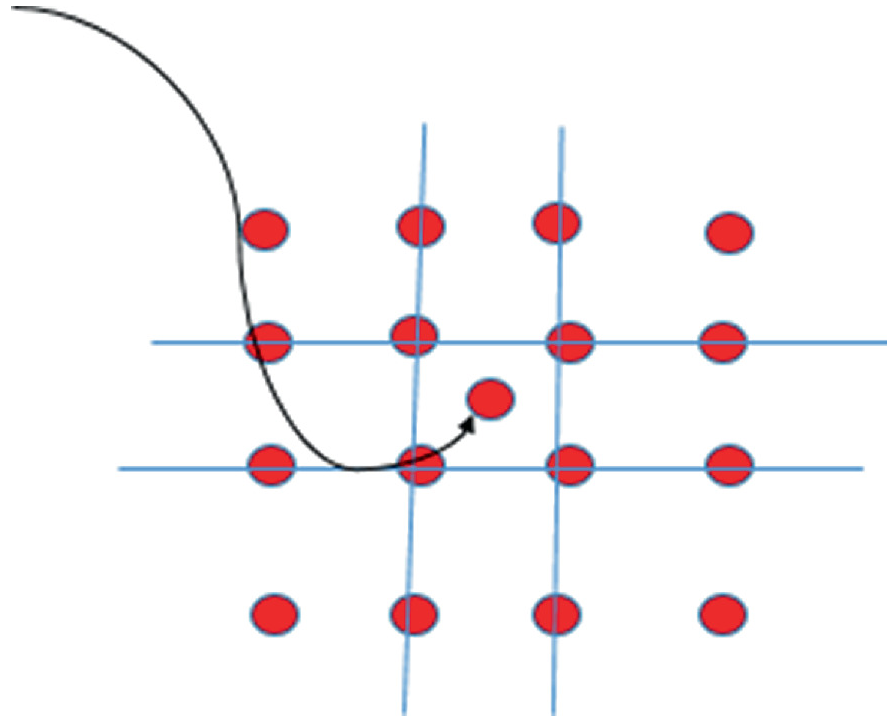


Fig. 3.10 Distortion of lattice due to interstitial (Avner, 1997)

Dislocation

Dislocation is a disturbed region between two substantially perfect parts of a crystal. Edge dislocation is created when an extra plane of atoms is inserted in the middle of the crystal. By convention, a positive dislocation has an extra plane of atoms in the upper plane, whereas in negative dislocation has an extra plane of atoms in the lower plane. The atoms in the upper plane are under compression for a positive dislocation, whereas the lower plane is under tension. The screw dislocation is so named because of the spiral surface formed by the atomic planes around the screw-dislocation line. The dislocation line produces compressive stress below the dislocation and tensile stresses above it and disturbed region in the lattice structure (Fig. 3.11).

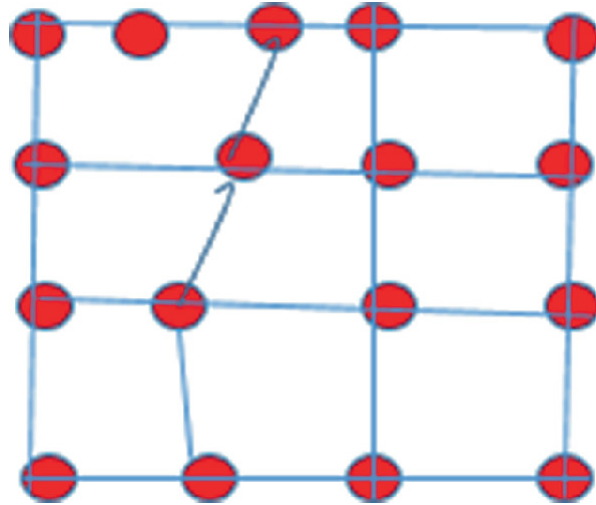


Fig. 3.11 Crystal imperfections (edge dislocation) (Avner, 1997)

Macrodefects

Defects that may result from solidification that is large enough to be visible to the naked eye are called macro defects. The most common macro defects are 1. Shrinkage cavity 2. Porosity 3. Hot Tears.

With few exceptions, liquid metals undergo a volume contraction due to solidification. The decrease in volume may be as much as 6 percent. If the entire exterior of the casting should solidify first, the decrease in volume of the interior during solidification will result in a large shrinkage cavity at the mid-section (Fig. 3.12).

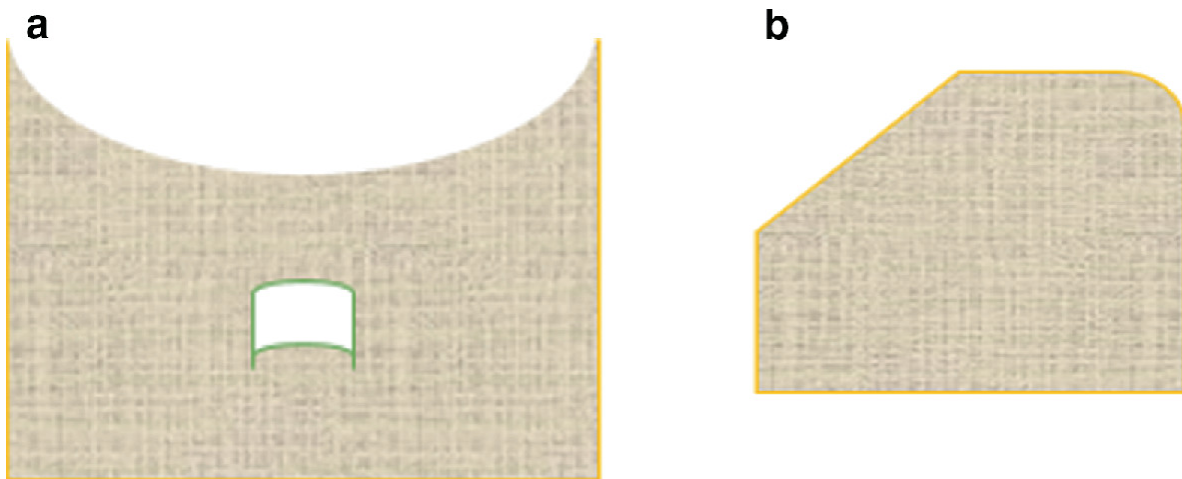


Fig. 3.12 a Shrinkage cavity and **b** Porosity (Avner, 1997)

Porosity or blowholes occurs whenever gases are trapped in the casting. Air may be entrapped in the casting by the sudden metal rush during pouring. Since gases are generally more soluble in liquid metal than solid, dissolved gases may be liberated during solidification. Gases may also be produced by the reaction of the liquid metal with volatile substances, such as moisture in the mold. Porosity may be greatly reduced by proper venting of the mold and by not unduly compacting the sand. Hot tears are cracks due to heavy shrinkage strains set up in the solid casting after solidification. A common cause is the failure of the sand mold to collapse and allow the casting to contract. Hot tears may also result from the same non-uniform cooling conditions that give rise to shrinkage cavities.

3.4 Explain Various Aspects of Grain Size Including Measurement Methods (Avner, 1997) From Materials Science Point of View⁴

The size of grains in casting is determined by the relation between the growth rate (G) and the nucleation rate (N). If the number of nuclei formed is high, a fine-grained material will be produced; if only a few nuclei are formed, a coarse-grained material will be produced. The cooling rate is the most important factor in determining the nucleation rate, i.e., the grain size. Rapid cooling (Chill cast) will result in many nuclei forming and fine grain size, whereas, in slow cooling (sand cast or hot mold), only a few nuclei are included and will have a chance to grow, depleting the liquid before more nuclei can form.

Other factors that increase the rate of nucleation:

1. Insoluble impurities such as aluminum (Al) and Titanium (Ti) form insoluble oxides in steel.
2. They were stirring the melt during solidification, which tends to break up the crystals before they can grow very large.

The rate of G relative to N is greatest at or just under the freezing point. If the liquid is kept accurately at the freezing point and a tiny crystal

touches the surface (seed), the crystal will grow down into the liquid. If it is withdrawn slowly, a single crystal can be produced. In general, fine-grained material shows better toughness. They are harder and stronger than coarse-grained material.

In the individual casting process, where a hot liquid is in contact with an originally cool mold, a temperature gradient will exist in the liquid. The outside is at a lower temperature than the center and starts to solidify first. Thus many nuclei are formed at the mold wall and begin to grow in all directions. They soon run into the side of the mold and each other so that the only unrestricted direction for growth is toward the center. The resulting grains are elongated columnar ones perpendicular to the surface of the mold. Next to the mold wall, where the cooling rate is fast, the grains are small, while toward the center, where the cooling rate is much slower, the grains are larger and elongated. If the mold has sharp edges, a plane of weakness will develop from this corner because both gaseous and solid impurities tend to concentrate along this plane. Such castings may cause internal rupture during rolling or forging operations. It is a good casting design to provide the mold with rounded corners to avoid a thin plane.

Grain Size Measurement

The 3 basic methods for grain size estimation recommended by the ASTM are:

1. Comparison Method
2. Intercept (or Heyn) Method
3. Planimetric (or Jefferies) Method.

Comparison Method

The image of the microstructure projected at a magnification of $100\times$ is compared with a series of graded standard grain-sized charts (ASTM E112-63). By trial and error, a match is fixed. The metal's grain is then designated by a number corresponding to the index number of the matching chart. Match showing a mixed grain size are rated similarly. It is customary in

many cases to report the grain size in terms of two numbers denoting the approximate percentage of each size present. The comparison method is most convenient and sufficiently accurate for specimens of equiaxed grains. The ASTM grain-size number (n) may be obtained as follows:

$$N = 2^{n-1} \quad (3.1)$$

N is the number of grains observed per square inch at $100 \times$ magnification.

Footnotes

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4. Bonds in Solids

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

4.1 Explain Basic Concept of Bonds in Solids

(Theraja, 2000) Applicable to Biomaterial¹

Bonding is the interaction between the atoms to form molecules by rearranging the electron in the atom to achieve a stable configuration.

The principal types of bonding in solids:

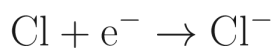
1. Ionic bonding
2. Covalent bonding
3. Metallic bonding
4. Dipole Bond (Van der Waals Bond).

Ionic Bonding

The bond between two atoms by transferring electrons is called an ionic bond.

These bonds are formed due to the electrostatic attraction between two stable ions.

It was considering NaCl formation. Na has the atomic number 11. So, its outermost shell has 1 electron. Where Cl has an atomic number of 17, its outer electron is 7. Therefore, if Na can give 1 electron and Cl can have 1 electron, both can have filled up their octate to be stable. But when Na gives 1 electron, it becomes ion Na^+ , and when Cl receives 1 electron, it becomes ion Cl^- . These two ions form bonds due to strong electrostatic force, i.e., NaCl.



Covalent Bonds

The bond between two atoms by sharing valence electrons is called a covalent bond. This bonding force arises due to the presence of shared electrons. In a covalent bond, electrons are shared by both atoms; the electrons do not become the exclusive property of any atom as in an ionic bond. Considering the case of Cl atoms. Each Cl atom has 7 valence electrons. The covalent bond is established between the two atoms because each contributes one electron, and the two atoms share the electron pair. Each has 8 electrons in its valence shell, thereby achieving stability.

A double or triple covalent bond is said to be formed when more than one pair of electrons is shared between two atoms (Fig. 4.1).

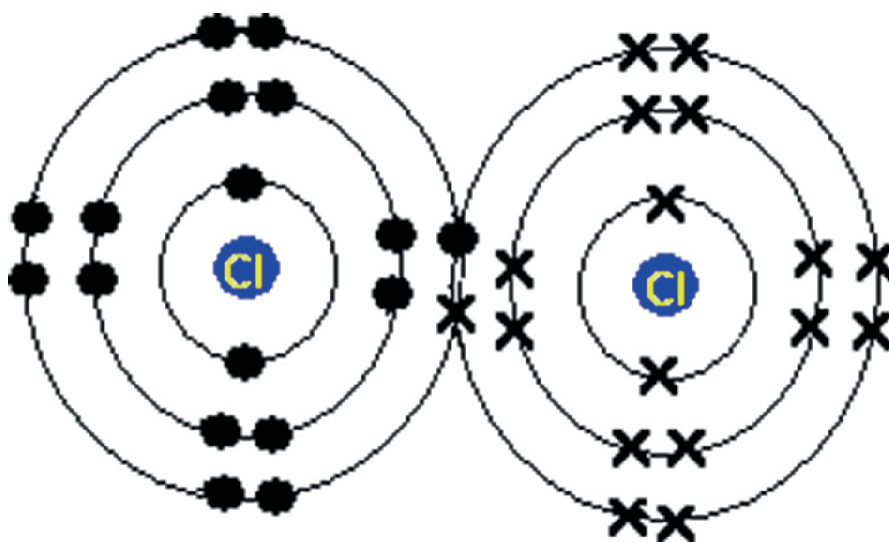


Fig. 4.1 Chlorine–chlorine covalent bond

Metallic Bond

Such a bond results from sharing a variable number of electrons with a variable number of atoms. Such bonds hold the atoms together in metals and their alloys. Each atom loses its valence electrons in metals and becomes a positively-charged ion. These free and mobile electrons form a kind of electron cloud or gas that permeates all atoms. It may look upon metal consisting of an array of closely-packed ions immersed in a sea of free electrons. The valence electrons are not bonded directly to an individual atom. Still, they move freely in the sphere of influence of other atoms and are bound to different atoms at different times.

A metallic bond may be considered an unsaturated covalent bond due to the electrostatic attraction between the negative electron cloud and positive

ion cores. The cohesion of a metallic crystal is due to the attraction of the positive nuclei and the valence electrons pressing between them. The metallic bond is comparatively weaker than the ionic and covalent bonds called saturated bonds (Fig. 4.2).

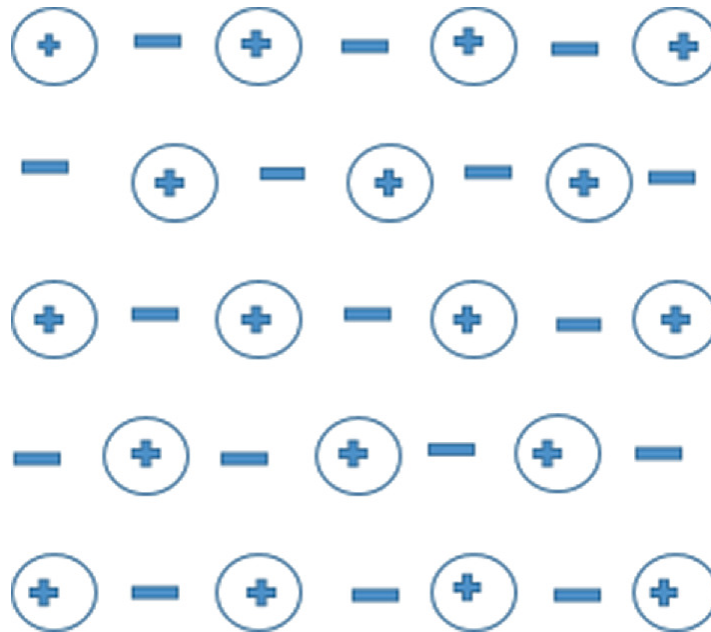


Fig. 4.2 Metallic bond (Theraja, 2000)

Dipole Bonding

This bonding is formed by the weak Van der Waal's forces of attraction, which exist between various atoms.

The net charge is zero for neutral atoms and molecules with filled shells, and there are no unpaired valence electrons available for sharing. Therefore, there is no opportunity for ionic, covalent and metallic bonding. For example, all inert gases have filled shells. The binding between inert gas atoms is quite weak. The attractive interaction between these inert gas atoms is due to the formation of induced dipoles. At some instant, the electron cloud of a given inert gas atom is slightly distorted due to random fluctuations or reduced thermal agitation, which means there are more electrons in one part of the atom than in another.

As a result, a dipole is formed. This dipole produces an electric field that acts on neighbouring atoms, inducing them to form dipoles. The resulting dipole-induced dipole attraction is known as Van der Waal's

interaction. Some molecules are permanent dipoles. The resulting dipole–dipole interaction contributes to cohesion between these molecules.

For example, hydrogen bonding. When it is bound to an electronegative element such as oxygen or nitrogen, the resulting bond is polarized; the OH and NH bond is slightly negative on the oxygen and nitrogen end side, respectively, while the hydrogen end is slightly positive (Fig. 4.3).

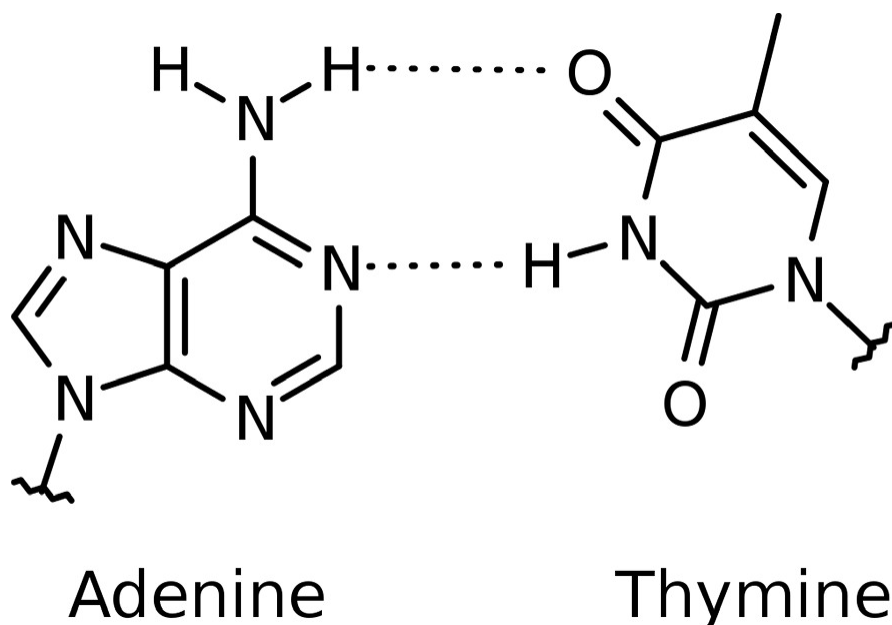


Fig. 4.3 Dipole–dipole bonding Robiul, 2000

Characteristics of Ionic Solids

- (i) Such solids usually have a crystalline structure. Their components are ions, not molecules. For example, each Na^+ ion is surrounded by 6 evenly spaced negative Cl^- ions in a NaCl crystal.
- (ii) Such solids are hard and brittle.
- (iii) Powerful electrostatic forces between the ions in the crystal lattice of an ionic solid. Consequently, considerable energy is required to overcome these forces and break down the crystal lattice. i.e., such solids have high melting and boiling points.
- (iv) Ionic solids are good insulators. There is no electronic conduction between the electrons because the electrons are tightly bound in the

filled shells of the two types of ions involved. However, there are some charge carriers while in solutions. Since ionic mobility increases with temperature, the electrical consistency of ionic solids also increases with the temperature, whereas metals whose electrical conductivity decreases with a temperature rise.

- (v) Ionic solids are quickly soluble in solvents like water (H_2O) and liquid ammonia (NH_3) because their molecules interact strongly with the crystal ions.
- (vi) Ionic reactions are practically instantaneous (i.e., precipitation). For example, Cl^- ions present in NaCl and BaCl_2 give a white precipitate of AgCl as soon as Ag^+ ions in the form of AgNO_3 solution are mixed.

Characteristics of Covalent Solids

- (i) Covalent compounds may be solids, liquids or gases. At normal temperature and pressure, they exist as gases or liquids. Those substances which have high molecular weights exist as solids. For example, Cl (molecular weight = 71) is gas, Br (molecular weight = 160) is liquid whereas I (molecular weight = 254) is a solid.
- (ii) Those in which small molecules are held together by weak forces, such crystals are soft and easily feasible. Examples are: (sulphur and iodine).
- (iii) Each atom is united with the other by covalent links, forming giant molecules. Examples are diamond and silicon carbide. In a diamond, each atom is united by covalent bonds with neighbouring carbon atoms held at the corners of a regular tetrahedron.
- (iv) Those which consist of separate layers such as graphite. Here, carbon atoms are arranged in regular hexagons in flat parallel layers, such that the neighbouring atoms link each atom. However, there is no strong bonding between different layers, i.e., they are easily separable. This is the cause of the softness and lubricating action of graphite.

- (v) Since covalent bonds are not as powerful as ionic bonds, covalent compounds have a comparatively low melting and boiling point.
- (vi) All covalent crystals are insulators because no electrons are available for conduction. However, some covalent crystals like those of diamond are excellent insulators, whereas others like Germanium (Ge) are semiconductors.
- (vii) Covalent compounds are soluble in non-polar solvents such as Benzene and Carbon Tetrachlorides.

Metallic Compounds Characteristics

- (i) They have a crystalline structure.
- (ii) Their electrical conductivity is extremely high due to the availability of an unlimited number of free electrons.
- (iii) Since metallic bonds are not very strong, such solids usually have moderate to high melting temperatures.
- (iv) They have a high thermal conductivity due to free electrons that serve as heat carriers.
- (v) Since free electrons in a metal absorb light energy, all metals are opaque to light.

Dipole Solids

- (i) Dipole substances can be both crystalline and non-crystalline. Their functional units are molecules. Moreover, as these crystals are formed of elements with low atomic numbers, they have low densities.
- (ii) Such solids have low melting points because of weak molecular bonds from Van der Waal's forces.

- (iii) Because no valence electrons are available in such solids, they are good insulators.
 - (iv) They are usually transparent to light.
 - (v) They are soluble in both polar and non-polar liquids.
-

Footnotes

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5. Basic Materials Science

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

5.1 Describe Schematically The Types or Alloy i.e. Consitution of Alloy¹

See Fig. 5.1.

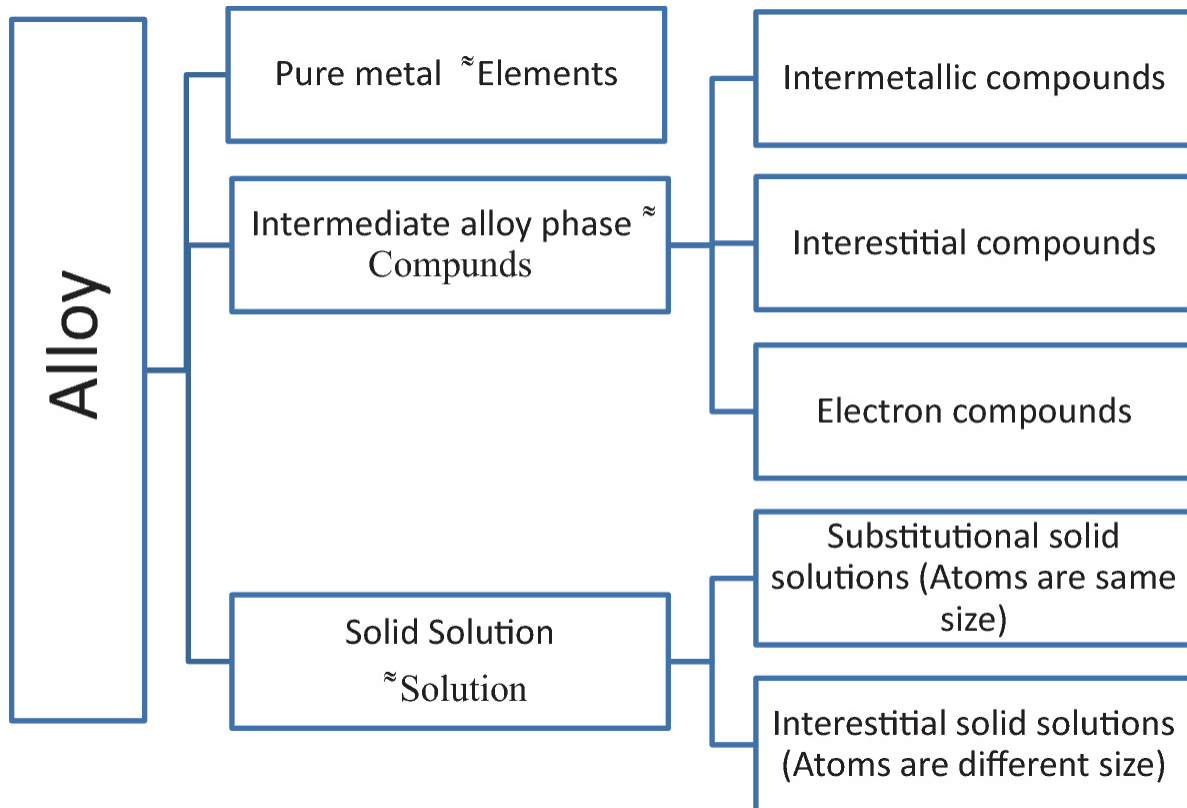


Fig. 5.1 Constitution of alloys (Avner, 1997)

5.2 Describe Basic Concept and Various Aspects of Alloy (Avner, 1997) For A Common Biomaterial

An alloy is a substance that has metallic properties and is composed of two or more chemical elements, of which at least one is a metal.

An alloy system contains all the alloys that can be formed by several elements combined in all possible proportions. If the system comprises two elements, it is called a Binary Alloy System. More elements are called a Ternary Alloy System. Taking only 45 of the most common metals, any combination of two gives 990 binary systems. Combinations of three give over 14,000 ternary systems.

Classification of Alloys

Alloys, maybe 1. Homogenous (Uniform) 2. Mixture.

If the alloy is homogenous, it will consist of a single phase; if it is a mixture, it will be a combination of several phases. A phase is anything that is homogenous and physically distinct. The uniformity of an alloy phase is not determined on an atomic scale and as the composition of each unit lattice cell but rather on a much larger scale. Any visible structure as physically distinct microscopically may be considered a phase. For most pure elements, the term phase is synonymous with the state. There is, i.e., for pure elements, a gaseous, liquid and solid phase. Some metals are allotropic in the solid state and will have different solid phases. When the metal changes the crystal structure, it undergoes a phase change since each type of crystal structure is physically distinct.

In the solid state, there are 3 possible phases:

- (i) Pure metal
- (ii) Intermediate alloy phase or compound
- (iii) Solid Solution.

If an alloy is homogenous (composed of a single phase) in the solid state, it can be only a solid solution or a compound. If the alloy is a mixture, it is then composed of any combination of the phases possible in the solid state. It may be a mixture of two pure metals, two solid solutions, two compounds, a pure metal, a solid solution, and so on. The combination may also vary in degree of fitness.

(i) **Pure Metal**

Under equilibrium conditions, all metals exhibit a definite melting or freezing point. The term under equilibrium conditions implies conditions of extremely slow heating and cooling. In other words, if any change occurs, sufficient time must be allowed for it to occur. A cooling curve plotted for a pure metal will show a horizontal line at the melting or freezing point.

(ii) **Intermediate Alloy Phase or Compound**

It will be simpler at this point to call it a compound. Most ordinary chemical compounds are combinations of positive and negative valence elements. The various kinds of atoms are combined in a delicate proportion, explained by a chemical formula. The atoms combined to form the molecule, the smallest unit with the compound's properties, are held together at a definite level. When a compound is created, the elements lose their identity and characteristic properties to a large extent—for example, NaCl and H₂O.

Most compounds, like pure metals, also exhibit a definite melting point within narrow temperature limits. Therefore, the cooling curve for a compound is similar to that for a pure metal. In reference to equilibrium diagrams, the intermediate alloy phases are phases whose chemical compositions are intermediate between the two pure metals and generally have crystal structures different from those of pure metals. The 3 most common intermediate alloy phases are.

1. Intermetallic compounds
2. Interstitial compounds
3. Electron compound.

1. **Intermetallic Compounds or Valency Compounds**

In many metallic systems, additional constituents are formed when compositions are intermediate between the two primary metals. These intermediate phases often exhibit properties entirely different from those of either of the constituent metals and other crystal structures completely different than either of the two metals. These are called intermetallics, such as Cu₃Al, CuZn, Mg₂Sn, Mg₂Pb and Cu₂Se. They show a bond with a mixed metallic/ionic or mixed metallic/covalent bond. These intermetallic compounds are generally formed between chemically dissimilar metals and combined according to chemical valence rules. They usually show poor ductility and poor electrical conductivity. They show non-metallic properties.

2. Interstitial Compounds

Compounds formed between the transitional metals such as Scandium (Sc), Titanium (Ti), Tantalum (Ta), Tungsten (W) and Iron (Fe) with H_2 , O_2 , C, B and N_2 . The word interstitial means between the spaces. The latter five (H, O, C, B, N) elements have relatively small atoms which fit into the spaces of the lattice structure of the metal. i.e., these compounds are called Interstitial compounds. Examples: TiC, TaC, Fe_4N , Fe_3C , W_2C , C_2N and TiH. The interstitial compounds are metallic, may have a numerous range of compositions, high melting points, and are extremely hard. Many of these compounds are useful in hardening steel and cemented-carbide tools.

3. Electron Compounds

Some intermediate corresponds which do not obey the normal rules of valency are called Electron compounds.

A study of the equilibrium diagram of copper, gold, silver, iron and nickel alloys with cadmium, Mg, tin, zinc and aluminum shows striking similarities. A number of intermediate phases are formed in these systems with similar lattice structures. Hume-Rothery first said that these intermediate phases are formed to exist at or near compositions in each system that have a definite ratio of valence electrons to atoms and are therefore called Electron compounds. For example, in the compound AgZn, the atom of silver has one valence electron. In contrast, zinc has two valence electrons, so the two atoms of the compound will have 3 valence electrons, or one electron-to-atom ratio is 3:2.

In the compound Cu_9Al_4 , each atom of copper has one valence electron and each atom of aluminum 3 valence electrons. The 13 atoms that make up the compound have 21 valence electrons or an electron-to-atom ratio of 21:13. For calculation, iron and nickel atoms are assumed to have zero valences. Many electron compounds have solid solutions resembling a wide range of composition, high ductility, and low hardness (Table 5.1).

Table 5.1 Electron compounds (Avner, 1997)

Electron-to-atom ratio = 3:2 BCC structure	Electron-to-atom ratio = 21:13 Complex cubic structure	Electron-to-atom ratio = 7:4 CPH structure
AgCd	Ag ₅ Cd ₈	AgCd ₃
AgZn	Cu ₉ Al ₄	Ag ₅ Al ₃
Cu ₃ Al	Cu ₃₁ Sn ₈	AuZn ₃
AuMg	Au ₅ Zn ₈	Cu ₃ Si
FeAl	Fe ₅ Zn ₂₁	FeZn ₇
Cu ₅ Sn	Ni ₅ Zn ₂₁	Ag ₃ Sn

Mixture: When two or more substances are mixed but not combined chemically is called a mixture.

Solution: A solution is a homogenous mixture of two or more substances.

Any solution is composed of two parts: a solute and a solvent. The solute is the minor part of the solution or the material dissolved, while the solvent is the major portion of the solution. It is possible to have solutions involving gases, liquids or solids as either the solute or the solvent. The most common solution involved water as the solvent, such as sugar or salt dissolved in water.

There are 3 possible conditions for a solution:

1. Unsaturated
2. Saturated
3. Super-saturated.

If the solvent is dissolving less of the solute than it could dissolve at a given temperature and pressure, it is said to be Unsaturated. If it dissolves a limiting amount of solute, it is called saturated. Suppose it dissolves more of solute than it should under equilibrium conditions; the solution is supersaturated. The latter condition may be accomplished by working on the solution, such as stirring or preventing equilibrium conditions by rapidly cooling the solutions. The supersaturated condition is unstable and given enough time or a little energy, the solution tends to become stable or saturated by rejecting or precipitating the excess solute.

The amount of solute the solvent may dissolve is generally a function of temperature. (with pressure constant) and usually increases with increasing temperature.

Solid Solutions

When a number of metals dissolve in each other, it is called solid solutions. A solid solution is a solid-state solution of one or more solutes in a solvent. Such a mixture is considered a solution rather than a compound when the crystal structure of the solvent remains unchanged by the addition of the solutes and when the mixture remains in a single homogenous phase. This often occurs when the two elements (generally metals) are closed on the periodic table. Conversely, a chemical compound is generally a result of the non-proximity of the two metals involved on a periodic table.

Footnotes

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6. Phase Diagrams

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

6.1 Describe Basic Concept of Phase Diagram (Avner, 1997) for Common Biomaterial¹

The graphical representation of an alloy system is called a phase diagram, equilibrium diagram, or substitutional diagram.

Since the properties of a material depend to a large extent on the type, number, amount and form of the phases present and can be changed by allowing these quantities, it is essential to know 1. The conditions under which these phases exist. 2. The condition under which a phase change will occur is where all this information is usually obtained from the phase diagram.

To completely specify the state of a system in equilibrium, it is necessary to specify 3 independent variables. These externally controllable variables are temperature, pressure and composition. With pressure around to be constant at atmospheric value, the equilibrium diagram indicates the structural changes due to variation in temperature and composition. Ideally, the phase diagram will show the phase relationships under equilibrium conditions and conditions where there will be no change with time. Equilibrium conditions may be approached by extremely slow heating and cooling, allowing sufficient time if a phase change occurs. In actual practice, phase change tends to appear at slightly higher or lower temperatures, depending upon the rate at which the alloy is heated or cooled. Rapid variation in temperature, which may prevent phase changes that normally occur under equilibrium conditions, will distort and sometimes limit the application of these diagrams. Conditions of equilibrium between phases in the binary alloy may be classified as:

1. Components completely soluble in the liquid state
 - a. Completely soluble in the solid-state (Type I)
 - b. Insoluble in the solid-state; Eutectic reaction. (Type II)
 - c. Partially soluble in the solid-state; Eutectic reaction. (Type III)
 - d. Formation of a congruent-melting intermediate phase (Type IV)

- e. The peritectic reaction (Type V).
2. Components partly soluble in the liquid state: The monotectic reaction (Type VI)
 3. Components are insoluble in the liquid state and insoluble in the solid state (Type VII)
 4. Transformations in the solid-state
 - a. Allotropic change
 - b. Order–Disorder
 - c. Eutectoid reaction
 - d. The peritectoid reaction.

Coordinate Phase Diagrams

Phase diagrams are usually plotted with temperature in degrees Centigrade or Fahrenheit as the ordinate and alloy composition in weight percentage as the abscissa. It is sometimes more convenient for certain scientific work to express the alloy composition in atomic percentage. The following formulas may make the conversion from weight percentage to atomic percentage.

$$\text{Atomic percentage } A = \frac{100x}{x + y (M/N)}$$

$$\text{Atomic Percentage } B = \frac{100y (M/N)}{x + y (M/N)}$$

where

M Atomic weight of metal A

N Atomic weight of metal B
 X atomic percentage of metal A
 Y atomic percentage of metal B.

Regardless of the scale chosen for temperature or composition, there will be no difference in the form of the resulting phase diagram.

Type 1—Two Metals Completely Soluble in the Liquid and Solid State

Since the two metals are completely soluble in the solid state, a substitutional solid solution will be the only type of solid phase formed. The two metals will generally have the same type of crystal structure and differ in atomic radii by less than 8% (Fig. 6.1).

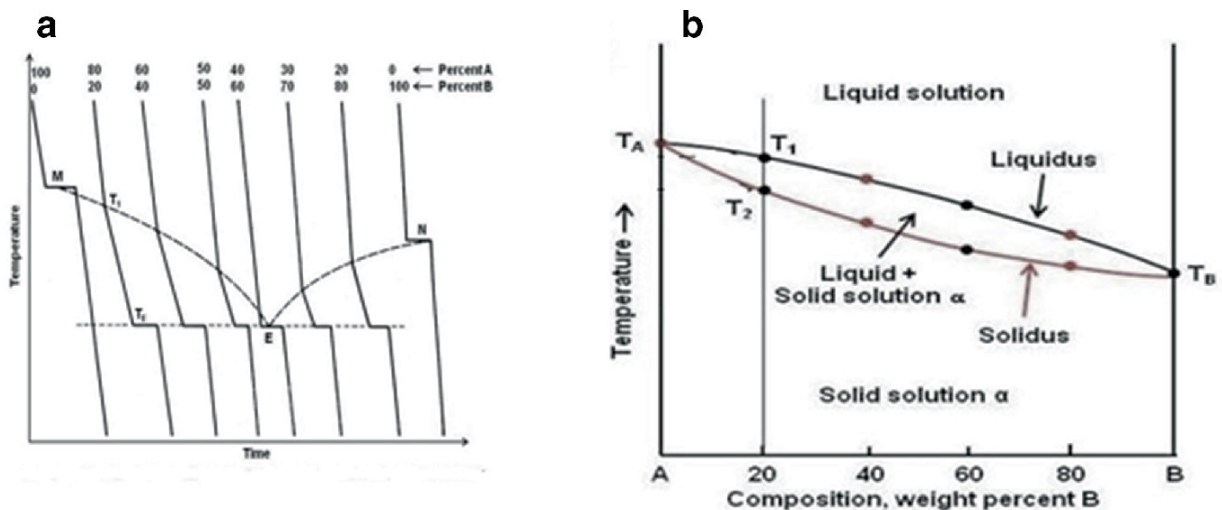


Fig. 6.1 A. Cooling curves; B. Phase diagram of two metals (completely soluble in the liquid and solid states) (Avner, 1997)

The result of running a series of cooling curves for various combinations or alloys between metals A and B, varying in composition from 100% A, 0% B to 0% A, 100% B, is shown in figure (A).

The cooling curves for the pure metals A and B show only a horizontal line because solidification's beginning and end occur at a constant temperature. However, since intermediate compositions from a solid solution, these cooling curves show two breaks or changes in slope. For an alloy containing 80A and 20B, the first break is at temperature T_1 , which indicates the beginning of solidification, and the lower break at T_2 indicates

the end of solidification. It is more possible to determine the metal phase diagram by plotting temperature versus composition Figure (B). T_A is plotted along the line since the left axis represents the pure metal A.

Similarly, T_B is plotted. Since all intermediate compositions are percentages of A and B, the % sign is omitted for simplicity. A vertical line representing alloy 80A–20B is drawn, and T_1 and T_2 from figure (B) are plotted along this line. The phase diagram consists of two points, two lines and three areas. The two points, T_A and T_B , represent the freezing points of the two pure metals.

The upper line, obtained by connecting the points showing the beginning of solidification, is called the liquidus line. The lower line, determined by connecting the points showing the end of solidification, is called the solidus line. The area above the liquidus line is a single-phase region; any alloy in that region will consist of a homogenous liquid solution. Similarly, the area below the solidus line is a single-phase region, and any alloy in this region will consist of a homogenous solid solution. Labeling equilibrium diagrams to represent solid solutions and sometimes intermediate alloys with Greek letters is common practice. In this case, the solid solution is alpha (α). Uppercase letters such as A and B represent pure metal. Between the liquidus and solidus lines, there exists a two-phase region. Any alloy in this region will consist of liquid and solid solutions.

Specification of temperature and composition of an alloy in a two-phase region indicates that the alloy consists of a mixture of two phases but does not give any information regarding this mixture. It is sometimes desirable to know the chemical composition and relative amounts of the two present phases. To determine this information, it is necessary to apply two rules (Fig. 6.2).

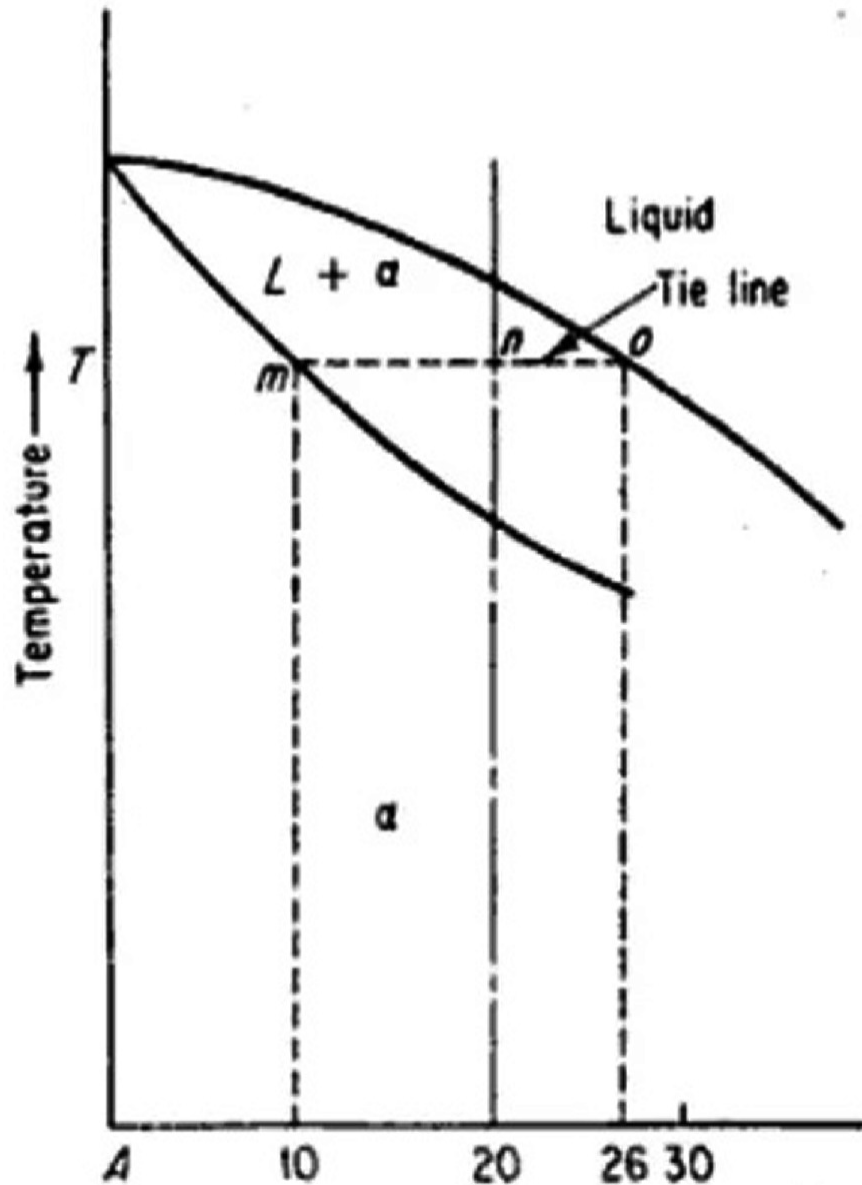


Fig. 6.2 Phase diagram (Two phase region at temperature T) (Avner, 1997)

Rule 1—Chemical Composition of Phases

To determine the actual chemical composition of the phases of an alloy in equilibrium at any specified temperature in a two-phase region, drawing a horizontal line, called a Tie-line, to the field's boundaries. These points of intersection are dropped to the baseline, and the composition is read directly. Figure (c) considers the alloy composed of 80A–20B at T temperature. The alloy is in a two-phase region. Applying Rule 1, draw the tie line m_0 to the field's boundaries. Point m, the intersection of the tie line

with the solidus line when dropped to the baseline, gives the phase composition at the boundary. In this case, the phase is a solid solution α of composition 90A–10B. Similarly, when dropped to the baseline, point O will give the composition of the other phase constituting the mixture, in this case, the liquid solution of composition 74A–26B.

Rule 2—Relative Amount of Each Phase

To determine the relative amount of the two phases in equilibrium at any specified temperature in a two-phase region, draw a vertical line representing the alloy and a horizontal temperature line to the field's boundaries. The vertical line will divide the horizontal line into two parts whose lengths are inversely proportional to the number of phases present. This is also known as the lever rule. The point where the vertical line intersects the horizontal line may be considered the fulcrum of a lever system. The relative lengths of the lever arms multiplied by the amounts of the phases present must balance. In fig (c), the vertical line representing alloy 20B divides the horizontal tie line into m_n and n_o . If the entire length of the tie line m_o is taken to represent 100% or the total weight of the two phases present at temperature T , the lever rule may be expressed as:

$$\begin{aligned} \text{Liquid (\%)} &= \frac{m_n}{m_o} \times 100 \\ \alpha (\%) &= \frac{n_o}{m_o} \times 100 \\ \therefore \text{Liquid (\%)} &= \frac{10}{16} \times 100 = 62.5\% \\ \therefore \alpha (\%) &= \frac{6}{16} \times 100 = 37.5\% \end{aligned}$$

from the figure (d).

To summarize both rules, the alloy of composition 80A–20B at the temperature T consists of a mixture of two phases. One is a liquid solution of composition 74A–26B constituting 62.5% of all the material, and the other is a solid compound 90A–10B constituting 37.5% of all material.

Equilibrium Cooling of a Solid-Solution Alloy: The very slow cooling under equilibrium conditions, diffusion will take place, and all the solid

solutions will be uniform composition. There are only grains and grain boundaries. There is no evidence of many chemical composition differences inside the grains, i.e., indicating that diffusion has made the grain homogenous.

Diffusion: Diffusion is a mass transport process that involves the movement of one atomic species into another and takes place in the gaseous, liquid and solid states for all classes of materials. It occurs by random atomic jumps from one to another.

There are three methods by which diffusion in substitutional solid solutions may occur.

1. The vacancy mechanism
2. Interstitial mechanism
3. Atom interchange mechanism.

6.2 Describe Basic Concept of Various Phases for a Common Biomaterial (The Iron-Iron Carbide Equilibrium Diagram (Avner, 1997))²

Ingot Iron: Iron ingots are a nearly pure form of iron.

The Iron–iron Carbide Equilibrium Diagram

Typically, ingot iron analysis is

C → 0.012%

Mn → 0.017%

Ph → 0.005%

S → 0.025%

Si → Truce.

Common mechanical characteristics

Tensile strength → 40,000 Psi.

Elongation in z'' → 40%

Rockwell B Hardness → 30.

Depending upon the temperature, the allotropic metal iron can exist in various lattice structures. In Fig. 6.3, a cooling curve for pure iron has been displayed.

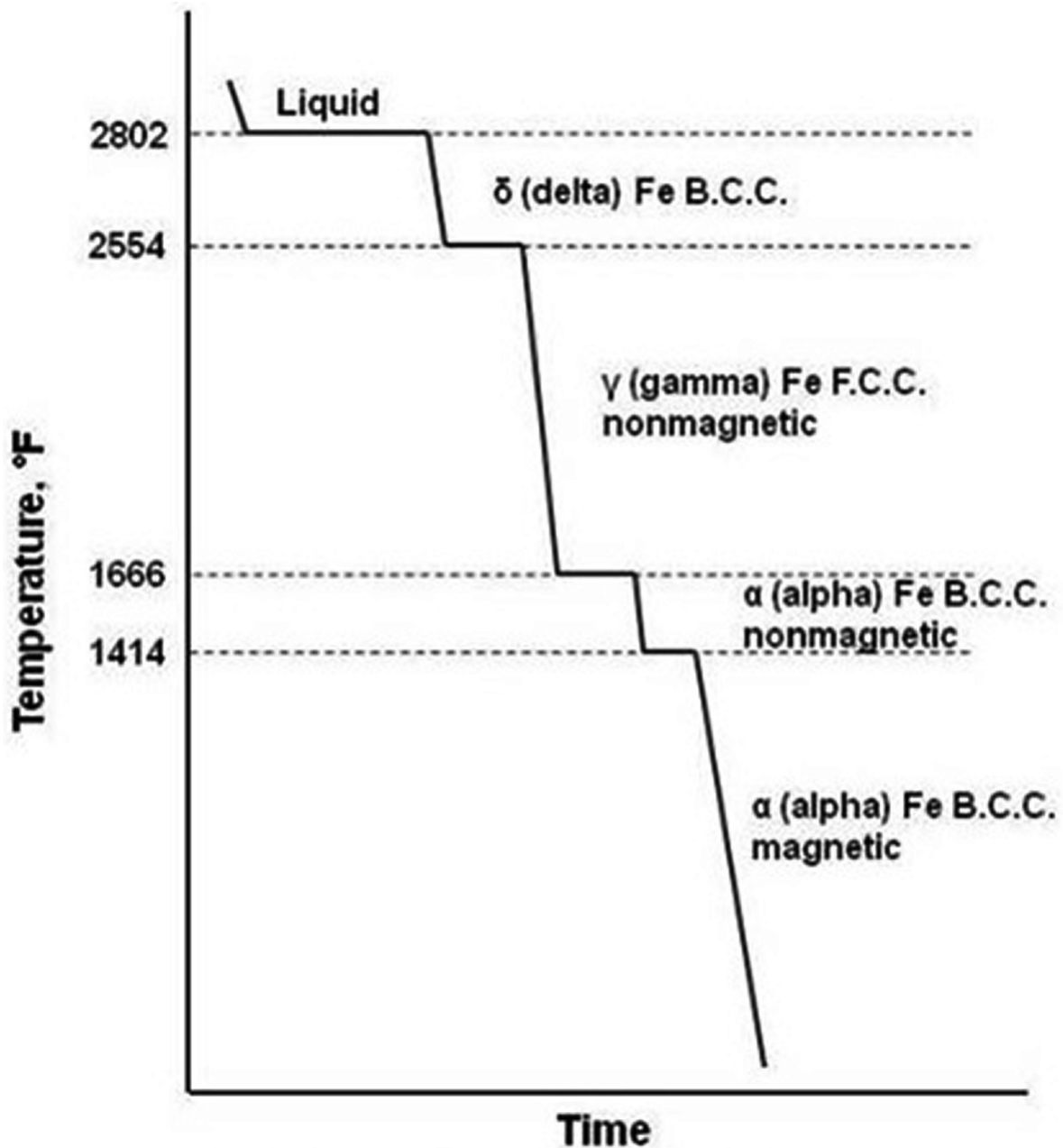


Fig. 6.3 Cooling curve of pure iron (Avner, 1997)

At 2800 °F, iron first solidifies in the BCC δ form. The atoms reorganize themselves into γ the FCC and nonmagnetic form after further cooling, which takes place at 2554 °F. Another phase change from FCC nonmagnetic iron to BCC nonmagnetic iron occurs when the temperature is reached 1666 °F. At 1414 °F, the iron finally starts to magnetic without altering its lattice structure.

Nonmagnetic α -iron was initially known as β -iron until later x-ray studies revealed that the lattice structure remained unchanged at 1414 °F. This magnetic transformation won't be taken into consideration in this discussion because it has no impact on how iron-carbon alloys are heated. When the iron is cooled, allotropic changes emit heat (exothermic), and when the iron is heated, they absorb heat (endothermic).

Wrought Iron

High-purity iron and slag make up the basic two components of wrought iron. Iron silicate makes up the majority of the slag. The iron contains physically distinct small and evenly dispersed slag particles. The slag and the iron are not chemically or functionally linked.

The iron is continually and quickly solidified because the slag is kept at a temperature significantly below the iron's freezing point. Numerous gases are dissolvable in the molten iron, but they become insoluble as the metal solidifies. This quick solidification releases gases in the form of numerous small explosions with enough force to break the metal into tiny pieces, which then fall to the bottom of the slag label. Shooting is the name given to this operation because of the noise the explosions make. The iron pieces stick together to form a sponge-like ball of iron globules coated in silicate slag because the iron is at a welding temperature and because the siliceous slag acts as a flux.

Chemical Analysis of Wrought Iron:

C $\rightarrow$ 0.06% (Generally below 0.08%)

Mn $\rightarrow$ 0.045% (Generally below 0.02%)

Si $\rightarrow$ 0.101%

Ph $\rightarrow$ 0.068%

S $\rightarrow$ 0.009%

Slag $\rightarrow$ 1.97% (By weight)

Wrought Iron as a composite material.
Tensile Strength → 48,000 – 50,000 Psi.
Yield Point → 27,000 – 30,000 Psi.
Elongation, the percentage in 8" → 18–25.
Reduction in area → 35–45%.

Cementite

Iron carbide, also known as cementite, has the chemical formula Fe_3C and 6.67% carbon by weight. Generally, it is a tough, brittle industrial substance with a greater compressive strength but a lower tensile strength. It is the diagram's toughest-looking structure. Orthorhombic crystals make up its structure.

Austenite

The term for the γ solid solution is austenite. It is an intercellular solid carbon solution in iron that has a γ (FCC) composition. 2% carbon is most soluble at 2065 °F (Point C). Tensile strength is 150,000 psi, elongation is 10% in 2", hardness is roughly Rockwell C 90, and toughness is high. These are the average characteristics. Normally, it is unstable at room temperature. Austenite can be obtained under specific circumstances at room temperature.

Ledeburite

The eutectic combination of cementite and austenite is ledeburite. At 2065 °F, it forms and has 4.3% carbon.

Ferrite

The term used to describe the α -solid solution is ferrite. It is a limited quantity of carbon soluble (BCC) iron in the form of an interstitial solid solution. Only 0.008% carbon dissolves at room temperature, and the maximum solubility is 0.025% carbon at 1333°F (Point H). It represents the diagram's softest-looking structure. Tensile strength of 40,000 psi, elongation of 40% in 2 inches, and toughness of less than Rockwell C 0 or less than Rockwell B 90 are considered average characteristics.

Pearlite

The eutectoid mixture with 0.8% carbon, known as pearlite (Point J), was developed at 1333 °F after a very slow cooling process. It is an extremely fine mixture of cementite and ferrite that resembles plates or lamellae. The majority of the wide range of eutectoids is composed of a white ferritic matrix containing thin cementite plates. The tensile strength of 120,000 psi, elongation of 20% in 2", and hardness of Rockwell C 20, Rockwell B95–100, or BHN 250–300 have been regarded as average characteristics. [Reference Fig. 7.7].

6.3 Classify Various Types of Steel with Alloying Effects [Avner, 1997] As A Common Biomaterial³

Classification of Steels

Several methods may be used to classify steels:

Methods of Manufacture

This method indicates Bessemer Steels, Open-Hearth Steels, Electric-Furnace Steel, Crucible Steel etc.

Use

Generally, this is the final for the steel, such as machine steel, spring steel, boiler steel, structure steel, or Tool Steel.

Chemical Composition

This approach reveals the approximate content of the key elements in the steel using a numbering system. The most common classification technique will be covered in more detail. The steel specifications are the result of a partnership between the Society of Automotive Engineers (SAE) and the America Iron and Steel Institute (AISI) with the goal of streamlining the process of satisfying the steel requirements of the American industry. The

1st digit of the 4 or 5 numerical designations indicates the type to which the steel belongs. Thus 1 shows carbon steel, 2 → nickel steel, 3 → nickel–chromium steel, etc. For simple alloy steels, the second digit represents an approximation of the percentage of the main alloying element. The final two or three digits typically represent the carbon content multiplied by 100. Hence, the symbol.

$$\underbrace{2}_{\text{Nickel}} \underbrace{5}_{\text{Steel}} \underbrace{20}_{5\% \text{Ni } 0.20\% \text{Carbon}}$$

In addition to the numerical information, the AISI configuration may also include a letter prefix to describe the steel's manufacturing process. The SAE specification no longer uses any letter prefixes and instead uses the same 4-digit numerical designations as the AISI specifications. AISI prefix letters.

B = Acid Bessemer Carbon Steel

C = Basic Open – Hearth Carbon Steel

Steels are sometimes classified by the broad range of carbon content, such as:

Low - carbon steel : up to 0.25%C

Medium - carbon steel : 0.25 to 0.55%C

High - carbon steel : Above 0.55%C

Effects of Small Quantities of other Elements

The iron-iron carbide equilibrium diagram was previously discussed under the assumption that only iron and iron carbide were present. Commercial plain carbon steels do, however, normally contain small amounts of other elements in addition to iron and carbon.

Sulfur

Typically, Sulphur content in commercial steels is kept below 0.05%. Iron sulphide is created when Sulphur and iron combine (FeS). Iron sulphide and iron, which tends to concentrate at the grain boundaries, combine to form a low-melting-point eutectic alloy. Steel has become brittle (hot-short) when it is forged or rolled at high temperatures because the iron sulfide eutectic

alloy melts, destroying the cohesion between grains and allowing cracks to form. The Sulphur content rises in the pre-machining steels to 0.08% to 0.35%. The increase in sulphide inclusions, which split the chips and lessen tool wear, is what makes the material more machinable.

Manganese (Mn)

All commercial plain carbon steels contain manganese in amounts ranging from 0.03 to 1.00%. Mn's purpose is to offset sulfur's negative effects. S is more likely to form MnS than FeS when Mn is present. The MnS may disperse inclusions throughout the structure or pass out the slag. It is instructed that Mn contains 2–8 times as much sulfur. The compound Mn_3C , linked to the iron carbide (Fe_3C) in cementite, is created when there is excess manganese compared to what is needed to form MnS. Mn also helps to ensure the stability of steel casting by deoxidizing liquid steel.

Phosphorus (P)

Typically, the phosphorus quantity is kept at or below 0.04%. This tiny amount tends to dissolve in ferrite, slightly boosting hardness and strength. 0.07% to 0.12% P enhances the cutting characteristics of some steels. P decreases ductility in larger concentrations, making steel more prone to cracking when cold worked and becoming cold-short.

Silicon (Si)

Silicon content ranges from 0.05% to 0.3% throughout most commercial steels. Si dissolves in ferrite, boosting steel's strength without significantly reducing ductility. The production of SiO_2 encourages the deoxidation of molten steel, which tends to increase casting soundness.

Footnotes

¹ Chapter 2 to 7 are written including compiled data for tables and redrawn schematics based on the references B. L. Theraja, 2000, "Modern Physics", S. Chand & Company Ltd. New Delhi, India, A. Pytel & F. L. Singer, 1995, "Strength of Materials", Haper & Row, New York, USA, J. P. Schaffer, A. Saxena, S. D. Antolovich, T. H. Sanders, and Steven B. Warner, 1999, "The Science and Design of Engineering Materials", WBC/McGraw-Hill, USA, Sydney H. Avner, 1997, "Introduction to Physical Metallurgy", Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, "Foundations of Materials

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7. Mechanical Properties and Testing

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

7.1 Describe Basic Mechanical Properties and Testing Aspects for a Common Biomaterial¹

Axial Force

The tension or compression that is applied to the section is measured by this component. A push is a compressive force that shortens the member, while a pull is a tensile force that elongates the member. P is a common way to indicate it.

Shear Force

These make up the resistance to sliding the exploratory section's portion to one side past the other. Usually, the shear force that results is denoted by the letter V.

Torque

The component measures the resistance to twisting the member and is commonly given the symbol T.

Bending Moment

These elements, which are frequently referred to as M_y or M_z , measure the member's bending stiffness about the Y and Z axes.

Stress

Stress is the force (the resistance to the applied force) per unit area.

$$\sigma = \frac{F}{A}$$

Stress that is constant or uniform is referred to as simple stress. Only if the result of the applied loads passes through the centroid of the cross-section can there be a uniform stress distribution.

Strength

A material's strength is determined by its capability to handle an applied stress without breaking down.

Stiffness

The ability of an elastic body to resist deformation when a force is applied is known as stiffness.

When power is applied, a property is said to be rigid if it does not bend or flex.

Elasticity

The ability of a material to resume its original shape following release of the stress that caused it to deform is known as elasticity.

Plasticity

The ability of a material to permanently deform under load is known as plasticity.

Tensile Stress and Compressive Stress

The stress condition that causes expansion is tensile stress. Compressive stress is a type of stress that acts on a material's center when it is applied. When a substance experiences compressive stress, it is said to be compressed. The forces that cause tensile and compressive stresses act perpendicular to the surfaces on which they act. Tensile and compressive stresses are often referred to as normal stress because of this.

Shearing Stress

Because shearing stress is produced by forces acting perpendicular to the area resisting the forces, it differs from tensile and compressive stress. Shearing stress may also be referred to as Tangential Stress for this reason. When the applied loads cause one body section to slide past its neighboring section, shearing stress is generated. The sign for shearing stress is

$$\gamma = \frac{V}{A}$$

Bearing Stress

Compressive and bearing stress are different in that bearing stress is a contact pressure between different bodies, while compressive stress is the internal stress brought on by a compressive force (Fig. 7.1).

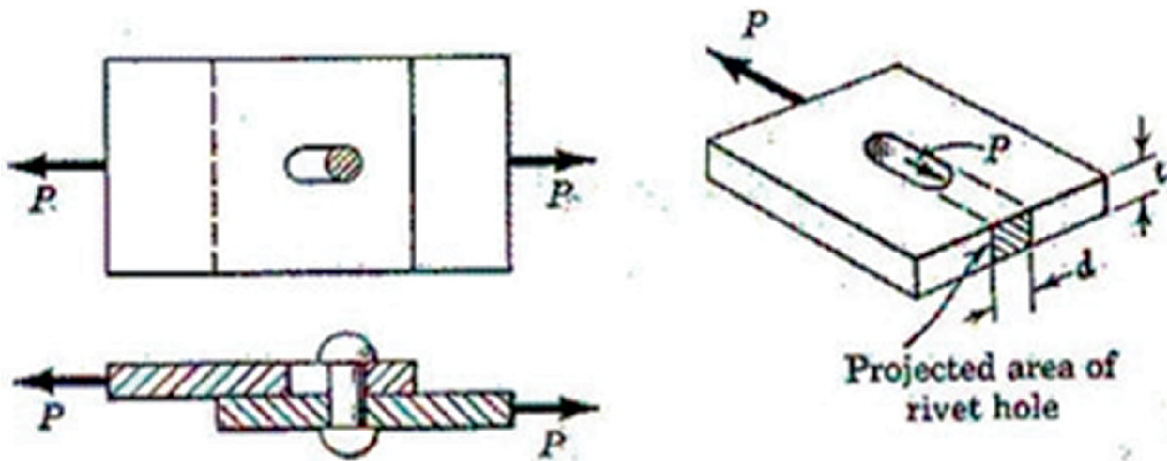


Fig. 7.1 Bearing stress (Pytel et al., 1995)

Residual Stress

Residual stresses are stresses that remain after the original cause of the stresses has been removed. These stresses remain in the part after the force has disappeared. Residual stresses always arise from non-uniform plastic deformation.

Hoop Stress or Girth Stress

The stress in the longitudinal section that resists the bursting force F in a thin-walled cylinder is called Hoop, Girth, or Circumferential Stress. This stress is usually called tangential stress because it acts tangent to the surface of the cylinder. A cylinder tank carrying gas or fluid under pressure is subjected to a tensile force that resists the bursting forces developed across longitudinal and transverse reactions.

Thermal Stress

Assume that a temperature deformation is allowed to happen innately because expansion joints will prevent the structure from experiencing any load or stress. However, in some circumstances, allowing these temperature deformations might not be possible. As a result, internal forces that oppose them are developed. Thermal stress refers to the stresses brought on by these internal forces. The magnitude of linear deformation (δ_T) is represented by:

$$\delta_T = \alpha.L.\Delta T$$

where

α coefficient of linear expansion, which unit is $m/^\circ C$

L original length

ΔT Temperature change.

Tension

Tension is the twisting of an object due to an applied torque. The result is the twisting of shearing stress. The maximum shearing stress:

$$\gamma_{max} = \frac{T.r}{J}$$

where

T torque

R radius of shaft

J Polar movement of inertia of the cross-section.

Flexural Stress

The stresses caused by the Bending Moment are known as Bending Stress or Flexural Stress.

Strain

Strain is the geometrical measure of change or deformation representing the relative displacement between particles in the material body. It is measured by the ratio between the change in dimension and the original dimension. If it is a 1-D change, then called elongation or longitudinal strain. If it is a 3D change, then called volumetric strain.

$$\epsilon = \frac{l}{L} [l = \Delta L = L_2 - L_1]$$

$$\text{or } \epsilon = \frac{\delta}{L} [\delta = \text{Elongation}]$$

Modulus of Elasticity

According to Hooke's Law, the relationship between stress and strain is constant, meaning that stress is directly proportional to the strain. The Modulus of Elasticity is the name given to this constant ratio. Tensile, compressive, and shear stresses are the three main types of stresses, and each has a corresponding modulus of elasticity.

Young's Modulus (E)

The modulus of elasticity in tension is called Young's Modulus (E), which is expressed as:

$$E = \frac{\sigma_E}{\epsilon_E} [\sigma_E = \text{Tensile stress}, \epsilon_E = \text{Tensile strain}]$$

Bulk Modulus (K)

The modulus compressibility (K) or Bulk Modulus ratio between hydrostatic pressure and relative volume changes.

$$\begin{aligned} \therefore K &= \frac{\text{stress}}{\text{volumetric strain}} = \frac{\sigma_C}{\epsilon_C} \\ &= \frac{\sigma}{\Delta V/V_0} [\Delta V = \text{change in volume}, V_0 = \text{original volume}] \end{aligned}$$

Modulus of Rigidity (G)

The modulus of elasticity in shear is the Modulus of Rigidity (G).

$$\therefore G = \frac{\text{Shear stress}}{\text{Shear strain}} = \frac{\tau}{\gamma} = \frac{\tau}{\delta_s/L}$$

where

τ shear stress

γ shear strain

δ_s shear deformation.

Relation Between 3 Moduli

Young's Modulus can also be calculated from Bulk Modulus and the Modulus of Rigidity as:

$$\frac{1}{E} = \frac{1}{9K} + \frac{1}{3G}$$

Poisson's Ratio (μ)

A transverse bar dimension decreases when it is lengthened by axial tension. The ratio of strains in these directions remains constant for stresses within the proportional limit.

When a rod is stretched by force applied at its ends, then the Poisson's ratio is the ratio of the lateral contracting strain to the elongation strain:

$$\therefore \mu = \frac{\text{lateral strain}}{\text{longitudinal strain}} = -\frac{G_y}{G_n} = -\frac{G_z}{G_u}$$

The negative sign indicates a decrease in transverse dimensions where ϵ_u is positive.

Stress–Strain Diagram

See Fig. 7.2.

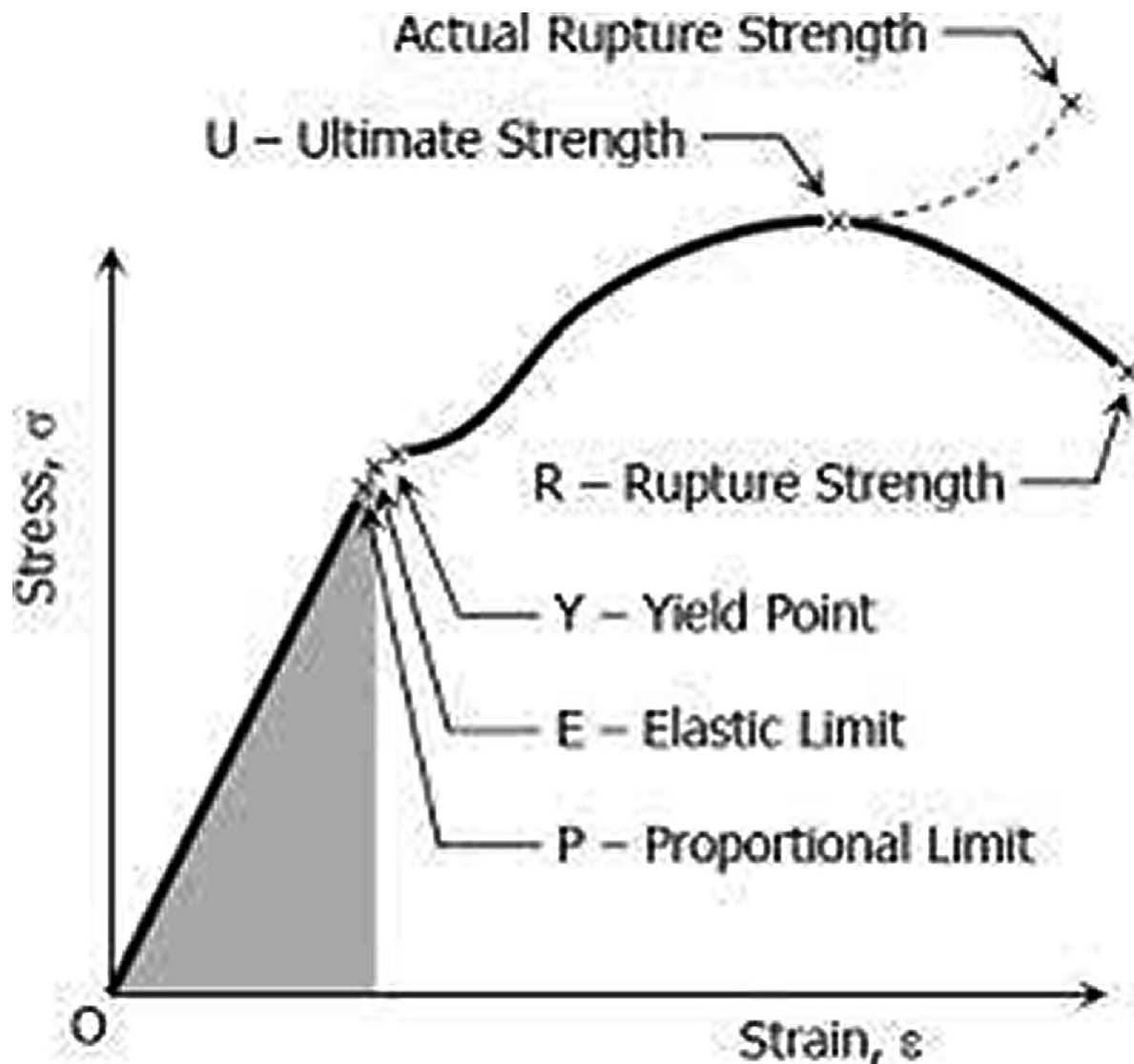


Fig. 7.2 Stress–strain diagram

Proportional Limit

Stress is proportional to strain, according to Hooke's Law. The diagram's proportionality stops at the proportional limit and does not continue beyond that point. The stress and strain are no longer proportional after this point. Therefore, any enhancement in stress will result in an equivalent enhancement in strain in this range, where stress and strain are proportional. The proportional limit is the strain at the proportionality point P's limit.

Elastic Limit

After a specific stress, the material will sustain its permanent deformation instead of returning to its original shape when unloaded. Therefore, the elastic limit is defined as the minimum stress of permanent deformation 1st occurs. For the majority of structural materials, the elastic limit has a numerical value that is very similar to the proportional limit.

Yield Point

The stress at which the material continues to deform or appreciable elongation or yield without increased load is called Yield Point. Where certain ductile materials, especially other grades of structural steel, exhibit this phenomenon, other steel alloys or materials do not.

Yield Strength

The stress at which a material displays a specific limiting deviation from the proportionality of stress or strain is known as the yield strength. The stress at which a material starts to deform plastically is known as the yield strength.

Ultimate Strength (Ultimate Tensile Strength)

The maximum amount of stress, compression, or shearing a material can withstand or sustain. The stress-strain diagram represents the maximum stress. When subjected to extreme stress, brittle materials fracture, whereas ductile ones continue to stretch. When the stress approaches the ultimate strength, Necking (localized deformation or ductile material forming a thin neck) occurs in the specimen, resulting in a smaller cross-section.

Rupture Strength (Breaking Strength)

The stress at failure after forming necking is the rupture strength. Because the rupture strength is calculated incorrectly by dividing the rupture load by the initial cross-sectional area, it is lower than the ultimate strength for structural steel. Necking is the cause of the mistake. A failure occurs; the materials stretch rapidly and simultaneously narrow to distribute the rupture load over a smaller area. If the rupture area is measured after a loss occurs and divided into the rupture load, a lower value of the actual failure stress.

While this is greater than ultimate strength, ultimate strength is typically regarded as the material's maximum stress. The ultimate and rupture strengths for brittle materials are equal.

Stress Concentration

A stress concentration is a phenomenon in which actual stress in a body becomes much more than the nominal due to abrupt changes in cross-sections and directional discontinuities.

Buckling

The failure mode of buckling is characterized by a structural member's sudden and unexpected failure under intense compressive stresses. The actual compressive stress is lower than the maximum compressive stresses the material can withstand at the point of failure. Failure resulting from elastic instability is yet another name for this failure mode.

Fracture

The separation of an object or material into two or more pieces under the action of stress.

Fatigue

Failure can happen when a material is exposed to cyclic loading, even if the applied stress is significantly lower than the material's ultimate strength. This mode of failure is known as fatigue.

Creep

When the load or stress is constant, strain increases with time. This phenomenon is known as creep. Creep is a time-dependent permanent deformation. It occurs due to long-term exposure to stress levels below the ultimate strength. Creep is the gradual deformation of a material over time while it is continuously stressed.

Modulus of Rupture (Flexural Strength)

When subjected to a bending load, a material can reject deformation. It is an aspect of brittle material mechanics. The maximum flexural stress experienced by the material at the rapture is represented by the flexural strength or modulus of the rapture.

Microhardness Test

Microhardness testing entails using tiny indenters. The range of test loads is 1–1000 gm. Microhardness tests are conducted using one of two types of indenters: 1. The 136° square-base Vickers diamond pyramid described previously, and 2. The elongated Knoop diamond indenter. Transverse angles of 130° and longitudinal angles of 172°30' were used to create the pyramid shape. The depth of indentation is about 1/30 of its length. The load divided by the area of the impression yields the Knoop hardness number. To convert the measured diagonal to a Knoop hardness number (HK), tables are typically available, or the following formula can be used:

$$HK = \frac{14.229 L}{d^2}$$

where

L applied load, kg

d length of long diagonal, mm.

Elongation

This is determined by filling together, after fracture, the specimen parts and measuring the distance between the original gauge marks.

$$Elongation (\%) = \frac{L_f - L_0}{L_0} \times 100$$

where

L_f Final gauge length

L_0 original gauge length, usually 2 inches.

The original gauge length must be specified in reporting the elongation percentage since the elongation percentage will vary with gauge length.

Reduction in Area

This is also determined from the broken halves of the tensile specimen by measuring the minimum cross-sectional area and using the following formula

$$\text{Reduction in area (\%)} = \frac{A_0 - A_f}{A_0} \times 100$$

where

A_0 original cross-sectional area

A_f Final cross-sectional area.

Ductility

The term “ductility” refers specifically to a substance’s capacity to deform when subjected to tensile stress. The substance’s capability to be stretched into a wire is frequently used to describe this. Ductile materials can withstand significant plastic deformation before breaking. It has mechanical characteristics.

Malleability

A material’s malleability is defined as its capacity to deform when subjected to compressive strength. This is frequently distinguished by the substance’s capacity to roll or hammer into a thin sheet. Lead (Pb) only exhibits malleability, whereas gold (Au) exhibits ductility and malleability.

Brittleness

Brittle materials are those that break easily and with little plastic deformation. When a material is exposed to external loads, the term “brittle” is used to describe it because it cannot absorb energy by “bending” but instead fractures (breaks into pieces). When under stress, brittle

materials are likely to fracture and have little tendency to deform (strain) prior to fracture, typically producing a mapping sound. There is typically little to no evidence of plastic deformation prior to failure, and it is typically applied to materials that fail in tension instead of shear.

Resilience

Resilience measures a material's ability to withstand energy in the elastic range. The material must have a strong yield strength and a low elastic modulus for high resilience. Resilience is calculated as the energy spent recovering from deformation divided by the energy needed to cause deformation. The ideal elastic material should have a ratio of one. However, because of the internal friction of natural materials, some energy is always lost as heat. Resilience is most impacted by temperature than by any other factor.

Hardness

A material's resistance to plastic deformation is quantified by its hardness. Typically, they are made by indentation (A pointed probe is called an indenter). The material is hard if significant forces are necessary to leave a permanent indentation mark. The phrase can also be used to describe stiffness, temper, or resistance to cutting, scratching, or abrasion. Indentation hardness can be measured using a variety of hardness tests, including Brinell, Rockwell, Microhardness, and Vickers Indentation.

Modulus of Resilience

The energy can be absorbed per unit volume in the elastic range without causing permanent deformation. The elastic range's area measures this energy under the curve (Fig. [7.3](#)).

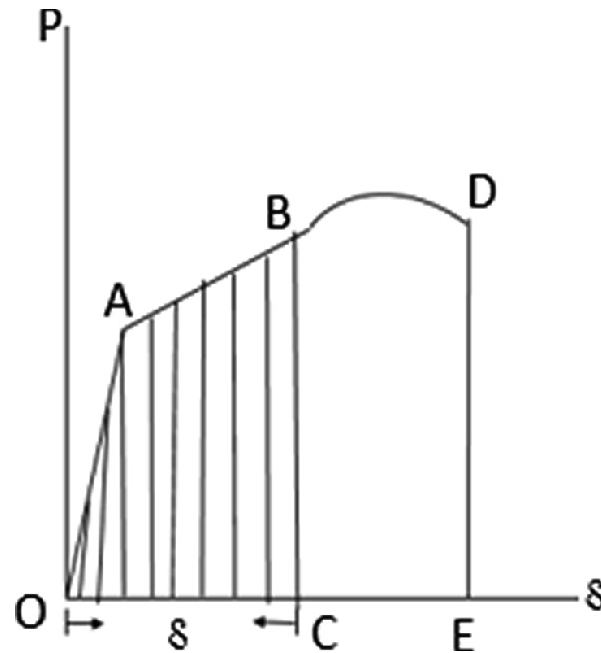


Fig. 7.3 Modulus of resilience (Pytel et al., 1995)

Vickers Hardness Test

Throughout this test, a square-based diamond-pyramid indenter with a 136° angle between opposing faces is used. The typical load range is 1 to 120 kg. The Brinell and Vickers hardness testers both work on the same fundamental principles, with the members being expressed in terms of loads and impression area. The shape of the indenter will cause a square impression to be left on the specimen's surface. It is determined how long the square's diagonal is. Using an ocular micrometer with movable knife edges mounted on a microscope. A counter calibrated in thousandths of millimeters displays the separation between knife edges. Vicker's pyramid hardness (HV) tables are typically available to convert the measured diagonal, or the formula shown below could be used.

$$HV = \frac{1.854 L}{d^2}$$

where

L applied load, kg

D Diagonal length of square impression, mm.

As a result of the latitude in applied loads, the Vicker tester uses to measure the hardness of very thin sheets and heavy sections (Fig. 1.17).

Toughness

The capacity of a material to hold onto energy during plastic deformation before breaking is known as toughness. The impact test will reveal the relative toughness.

Modulus of Toughness

The specific characteristic is known as the modulus of toughness, which measures the highest amount of energy per unit volume a material can withstand without fracture (The area under the entire stress–strain diagram). Since only a small portion of the total energy absorbed is elastic energy, which can be recovered when the stress is released, this is primarily a plastic range property. Brittle materials have low toughness because their plastic deformation prior to fracture is minimal.

Indentation

This test is typically carried out by directly or indirectly applying a known static load to the specimen while it is resting on a rigid platform, along with an indenter of fixed and known geometry. For a given load and indenter, the hardness is expressed by a number that is either inversely proportional to the indentation depth or proportional to the mean load applied to the entire indentation area.

Brinell Hardness Test

A hand-operated vertical hydraulic press intended to press a ball indenter into the test specimen typically makes up a Brinell hardness tester.

Brinell Hardness Number

The ratio of the load in kg to the impressed area in mm^2 is calculated from the following formula

$$HB = \frac{L}{\left(\pi D/2\right) \left(D - \sqrt{D^2 - d^2}\right)}$$

where

L test load, kg

D diameter of ball, mm.

d diameter of impression, mm.

The Brinell hardness number is immediately followed by the HB symbol without the suffix no. Indicates standard evaluation criteria with a ball of 10 mm in diameter and a load of 3000 kg applied for 10 to 15 s. In other cases, the hardness number and symbol HB are accompanied by numbers listing the test conditions in the following order: ball diameter, load, and loading duration. For instance, 75 HB 10/500/30 denotes a Brinell hardness of 75 calculated with a ball of 10 mm in diameter and a load applied for 30 s that weighs 500 kg. The Brinell hardness of a standard ball is approximately 500 HB. Using a tungsten carbide ball rather than a hardened steel ball can extend the scale's upper limit. Then, it is possible to travel for about 650 HB.

Rockwell Hardness Test

A direct-reading device based on differential depth measurement is used for this hardness test. A fixed minor load is applied before the test is completed by slowly raising the specimen against the indenter. The dial gauge displays this. After that, a loaded lever system applies the main load. The major load is excluded once the dial pointer has reached rest, and while the minor load is still in motion, the dial gauge can be used to read the Rockwell hardness number. Because the numbers on the dial gauge are arranged in reverse, a shallow impression on a hard material will produce a high no. A deep impression on a soft material will produce a low no.

The normal tester is for relatively thick sections, and the superficial tester is for thin sections. There are two types of Rockwell m/c. The minor load is 10 kg on the normal tester and 3 kg on the superficial. Indenters include hard steel balls 1/16, 1/8, 1/4 and 1/2 inch diameters and a 120°

conical diamond point. On the normal tester, major loads typically weigh 60, 100, and 150 kg, while on the superficial tester, they weigh 15, 30, and 45 kg. The “B” (1/16-inch Ball indenter and 100 kg load) and “C” (Diamond indenter and 150 kg load), both obtained with the standard tester Rockwell, are the two that are most frequently used. Rockwell is specified by “HR” after the letter designating the scale and before the hardness no. As an illustration, 82 HRB denotes a Rockwell hardness of 82 on the B scale. (100 kg load and a 1/16” ball).

Plastic Deformation

When a material is stressed below its elastic limit, a temporary deformation or strain results; once the stress is removed, the object returns to its original dimensions. When stressed past its elastic limit, a material experiences plastic or permanent deformation and cannot be forced back into its original shape. Slipping, twinning, or combining these two processes can result in plastic deformation.

Slip

Slip is a term used to describe a significant displacement of a crystal’s constituent parts concerning one another along specific crystallographic planes and in specific crystallographic directions. These particular crystallographic planes are called the slip planes or glide planes, and the preferable direction is called the slip direction.

Deformation By Slip

Let us say a single metal crystal is under tension stress that exceeds its elastic limit. In that case, it begins to elongate slightly before stopping. A step then appears on the surface to indicate the relative displacement of one part of the crystal to the other. Expanding the load will create a further step because it will cause mobility on a different parallel plane. It appears as though adjacent, thin pieces of crystal slid past one another like playing cards in a deck. Significantly greater stress is required for each additional elongation, which causes the appearance of another step—the point at which a sliding plane intersects the crystal’s surface. The material eventually fractures as the load is gradually increased. Investigations

revealed that sliding happened within the crystal's specific atomic planes and directions.

According to research into how the sliding plane is oriented to the applied stress, sliding occurs due to simple shearing stress. Two loads are produced by resolving the axial tensile load F in Fig. 3.1. One is a normal tensile load ($F_n = F \sin \theta$) perpendicular to the plane, and the other is a shear load ($F_s = F \cos \theta$) along the slip plane. The slip plane's area is $A / \sin \theta$ where A is the cross-section area perpendicular to F (Fig. 7.4).

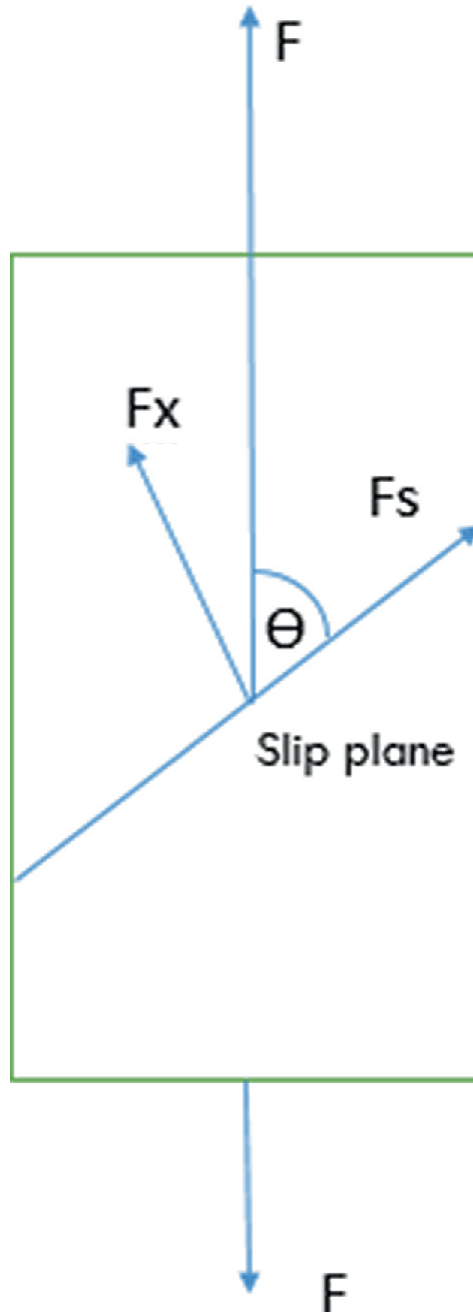


Fig. 7.4 Deformation by slip (Avner, 1997)

The resulting stress is:

Shear stress,

$$S_s = \frac{F \cos \theta}{A / \sin \theta} = \frac{F}{A} \cos \theta \cdot \sin \theta$$

$$\therefore S_s = \frac{F}{2A} \sin 2\theta \quad (7.1)$$

Normal stress,

$$S_n = \frac{F \sin \theta}{A / \sin \theta} = \frac{F}{A} \sin 2\theta \quad (7.2)$$

From Eq. (7.1), it is evident that the shear stress on a slip plane will be maximum when $\theta = 45^\circ$.

The shear direction on the slip plane is a more crucial factor in determining slip mobility. The direction in which the atoms are packed most densely wins, and this is where slip happens. The least amount of energy is needed for this. Closed-packed rows can pass each other off as less intelligent because they are farther apart than rows that are not closed-packed. Additionally, because the atoms are only held together by the free electron gas and not a direct bond, these densely packed rows of atoms could pass one another without breaking (Fig. 3.1a, b). Figure 3.3 shows the packing of atoms on a slip plane. The atoms are tightly packed in three directions, and these are also the directions where there would be easy slippage. In order to calculate the resolved shear stress (S_{rs}), the shear stress (S_s) on the slip plane must be resolved into the closest slip direction if it does not coincide with one of these simple slip directions. According to the diagram, the cosine of the angle (λ) connects the stresses, and the resolved shear stress is:

$$S_{rs} = \frac{F}{2A} \sin 2\theta \cos \lambda \quad (7.3)$$

According to research, when different axial stresses are applied, crystals of a given metal with different orientations will start to slip. The stress needed to start a slip is called Critical Resolved Shear Stress, whereas the critical resolved shear stress is constant. Slip cannot occur if other slip planes are either parallel to or perpendicular to the direction of applied stress; instead, the material will either fracture or undergo twinning deformation. The axial tensile load is maintained while deformation continues. The axis of tension is generally rotated by the sliding plane and sliding direction (Fig. 3.4).

Slip System

A slip system results from the alignment of a slip plane with a slip direction. The most crucial component of the slip system is the slip direction, which is always the densest atomic packing in the slip plane.

Slip in Different Lattice Structure

FCC materials have four sets of (111) planes and three densely packed (110) directions in each plane, giving rise to 12 possible slip systems. As a result, materials with this type of lattice structure (Silver, Gold, Copper, and Aluminum) are easily deformable, and a slip with critically resolved shear stress would be low. The (0001) plane, also known as the basal plane, is the only high-atomic-population plane present in the CPH metals (Cd, Mg, Co, and Ti), and it contains three closed-packed (112 0) atoms (Fig. 3.10). Compared to the FCC lattice, this structure has fewer slip systems, and its critical resolved shear stress is greater (Table 3.1). However, when the number of slip systems is constrained, the plasticity of the FCC structure is approached and surpassed by that of BCC metals. BCC metals lack a clearly defined sliding system and a close-packed plane because they have very few atoms per unit cell. The close-packed (111) direction is the slip direction. Slip plane identification is frequently challenging in BCC metals due to the heavy and erratic nature of the slip lines. The slip planes in BCC crystals have all been distinguished as planes 110, 112, and 123. The scarcity of a tightly packed plane and the surprisingly high critical resolved shear stress for slip are consistent (Table 3.1). Molybdenum, α -iron, and tungsten are examples of BCC metals that lack plasticity.

Twinning

Twinning is the process by which the atoms in a stressed portion of a crystal reorganize themselves to produce a mirror image of the original portion. Every atomic plane moves in the same direction but by a different amount depending on how far away it is from the twinning plane. The shear stress required for twinning is substantially greater than that for slip, which is typically negligible in many plastic deformations. Moreover, when the number of possible slip systems is significantly constrained, as in the case of hexagonal metals, twinning emerges as a significant deformation mode. Influence, thermal treatment, and plastic deformation are all potential causes of twinning.

Deformation by Twinning

Twining is a significant deformation in some materials, especially CPH metals. This could result in a significant change in shape or move potential slip planes into a better slip position. Twinning is the motion of atoms' lattice planes in a direction parallel to a chosen plane. The lattice is split into two rotationally symmetric, but not identical, parts. Each plane of atoms in a twinned region moves in proportion to how far away it is from the twinning plane, creating a mirror image across the twin plane. In Figs. 3.11 and 3.12, twinning is demonstrated in an FCC lattice (Fig. 7.5).

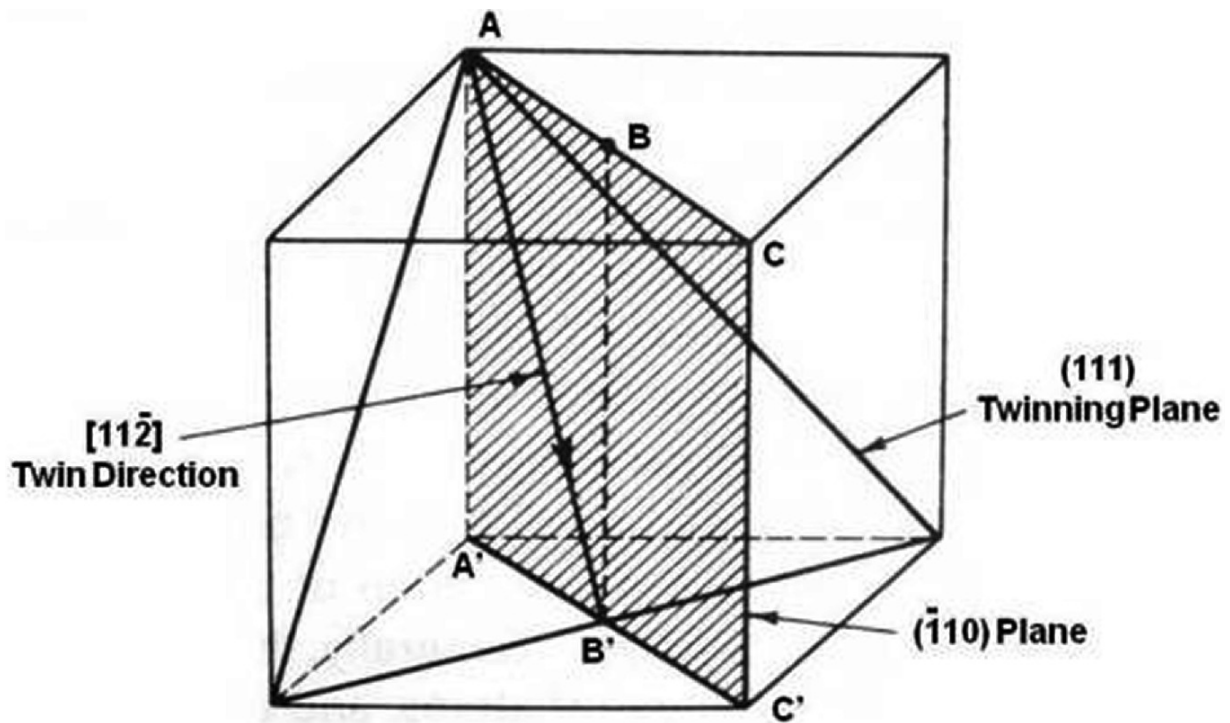


Fig. 7.5 Deformation by twinning (Avner, 1997)

In Fig. 3.11, the (111) twinning plane intersects the ($\bar{1}10$) plane along the line AB', the twin direction. The mechanism of twinning is shown in Fig. 3.12. The plane of the paper in the ($\bar{1}10$) plane, and many unit cells are taken together. Each (111) plane in the twin region moves in shear in the $[11\bar{2}]$ direction. The 1st one (CD) moves 1/3 of an interatomic distance; the 2nd one (EF) moves 2/3 of the interatomic distance, and the 3rd one (GH) moves an entire spacing.

Observe that a second atom (C') is located the same distance from the twinned plane but on the opposite side of a line perpendicular to the twin plane (AB') is drawn from atom A'. There is a mirror reflection of the untwinned portion of the crystal in the twinned region because this is true for all the atoms there. The orientation of the atoms or the spacing between atoms has changed because the atoms end up in interatomic spaces. The twinned region typically involves the movement of numerous atoms and manifests itself under the microscope as a broad line or band. The plane and direction for twinning are different from those for slip. The twin plane in FCC metal is the (111) plane, and the twin direction in the $[11\bar{2}]$ directions in BCC, it is the (112) plane and the [111] direction. The metallurgist is interested in two different types of twins.

1. Deformation or mechanical twins are mostly prevalent in CPH metals (Mg, Zn, etc.) and BCC metals (W, α -Fe, etc.)
2. FCC metals have the most annealing twins (Al, Cu, Brass, etc.). These metals have undergone previous processing followed by reheating. The alteration in the body's typical growth mechanism causes the twins to develop.

Slip Versus Twinning

Slip and Twinning differ in:

1. Amount of movement: Atoms in twinning move in fractional amounts depending on how far they are from the twinning plane, while those in slip move in whole numbers of interatomic spacings.
2. Microscopic appearance: Twinning appears as broad lines or bands, whereas slip appears as thin lines.
3. Lattice orientation: The lattice orientation changes very little during slip, and the steps are only apparent on the crystal's surface. There will not be any indication that someone fell if the steps are taken out by polishing. Moreover, reducing the steps by surface polishing in twinning will not eliminate the evidence of twinning because the twinned region has a different lattice orientation. The twinning region

can be seen using an appropriate etching solution keenly aware of orientational variations.

Fracture and Mechanism

A body under stress fractures when it splits into two or more pieces. Either brittle or ductile failure is used to describe it. With little energy absorption and plastic deformation, brittle fracture typically involves rapid crack propagation. Brittle fracture in single crystals is caused by cleavage along a specific crystallographic plane. Because the orientation of the cleavage plane varies from grain to grain in polycrystalline materials, the brittle-fracture surface appears granular. There were numerous small, elliptical submicroscopic cracks in the metal that led to failure in brittle materials. Even when the body of the material is subject to relatively low applied tensile stress, the sharpness at the tip of such cracks will result in a very high-stress concentration that may increase the theoretical fracture strength in this localized area and cause the crack to propagate. Due to its previous history of solidification or working, metal may have micro cracks. However, even a material that is initially sound can experience atomic-scale cracking.

Before the failure, there is significant plastic deformation well before ductile fracture. When a neck forms in a tensile specimen, the failure of most polycrystalline ductile materials manifests as a cup-cone fracture. In a tensile specimen, the fracture starts when a neck forms. Cavities start to form in the middle of the necked region as the fracture progresses. These internal cavities most likely develop at nonmetallic inclusions in most commercial metals. Highly pure metals are significantly more ductile than slightly less pure metals, which gives legitimacy to this belief. Due to persistently applied stress, the cavities combine to form a crack in the sample's midpoint. Perpendicular to the applied stress, the crack spreads outward toward the piece's surface. The fracture is completed quickly along a surface that forms a 45° angle with the tensile axis.

Cleavage: A crystal's splitting (fracture) on a crystallographic plane of the low index is called cleavage.

Slip, Twinning and Fracture

The proportion of the stresses needed for slip, twinning, and cleavage determines the deformation that can occur before fracture. Alloying, lowering temperature, and prior deformation all raise the critical resolved shear stress for the slip. Critical shear stress exists for twinning, and prior deformation makes it worse. Additionally, a specific plane has a critical normal stress for cleavage unaffected by previous deformation and temperature. Which Critical stress is easily surpassed first determines the process when stress is applied to a crystal. The crystal will slip or twin and exhibit some ductility if the critical resolved shear stress for slip or twinning is first reached. if the critical level of normal stress is nevertheless reached. The crystal will first cleave along the plane with little to no plastic deformation in mind.

Footnotes

¹ Chapter 2 to 7 are written including compiled data for tables and redrawn schematics based on the references B. L. Theraja, 2000, "Modern Physics", S. Chand & Company Ltd. New Delhi, India, A. Pytel & F. L. Singer, 1995, "Strength of Materials", Haper & Row, New York, USA, J. P. Schaffer, A. Saxena, S. D. Antolovich, T. H. Sanders, and Steven B. Warner, 1999, "The Science and Design of Engineering Materials", WBC/McGraw-Hill, USA, Sydney H. Avner, 1997, "Introduction to Physical Metallurgy", Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, "Foundations of Materials Science and Engineering", 2004, McGraw-Hill, 3 Ed, New York, USA and William D. Callister Jr. & David G. Rethwisch, 2009, "Materials Science and Engineering: An Introduction", 8th ed. John Wiley and Sons. NJ, USA.

8. Surface Engineering

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

8.1 Explain Various Aspects of Surface Engineering in Common Biomaterials¹

Wear

Wear is the removal of material from a solid surface by the action of another surface of material or friction.

The displacement and detachment of metallic particles from a metallic surface may be caused by, or the type of wear are:

1. Adhesive or metallic wear
2. Abrasion wear (a metallic or nonmetallic adhesive)
3. Erosion wear (moving liquids or greases).

If the critically resolved shear stress for slip or twinning is first reached, the crystal will slip or twin and show some ductility; however, if the limit of normal stress is crossed. The crystal will initially cleave along the plane with little to no consideration for plastic deformation. Since wear can rarely be avoided completely in most machinery applications, even with the best lubrication, using a hard metal and a relatively soft one is common.

Erosion

Erosion is a gravity-driven process that moves solids in their source and deposits them elsewhere.

Mechanism of Wear

Adhesive wear, also known as scoring, galling, seizing, and scuffing, is caused by small projections causing mechanical interference, with the relative motion of contacting surfaces enhancing reluctance to further mobility. If the driving force is adequate to keep the particles moving, the interlocked particles are distorted. They might be ripped off if they are made of brittle material. This results in the conclusion that avoiding metal-to-metal contact, enhancing toughness to resist early indentation, hardness

to resist tearing out of metallic particles, and surface smoothing to reduce projections will enhance wear resistance.

Abrasive wear results when a hard surface reigns over another surface or when hard particles glide or roll across one surface under pressure. The softer substance usually gets scratched or gouged by the abrasive particles from the tougher component. These strong particles may also puncture the softer metal, causing metallic particles to rip off. The toughness determines how the deformed metal can be torn off. As a result, the same qualities that affect adhesive wear also affect abrasive wear: hardness and toughness. Hardness is arguably the more significant of these two variables.

Galling

Surface damage arises between sliding solids, usually localized, roughening due to excessive friction.

In other words, galling is materially transformed from one metallic surface to another caused by movement and plastic deformation.

Factors Influence Wear:

1. Lubrication

Lubrication plays a significant role in wear resistance, particularly in adhesive wear. In “thick-film” lubrication, metallic contact is removed by a lubricating layer that is suitably thick, which minimizes metallic wear at the boundary. The degree of wear is influenced by speed, pressure, the makeup of the mating surfaces, and the effectiveness of the remaining oil film (where oil film cannot be continually maintained). Lubrication is frequently required or undesirable, such as when braking.

2. Heat

The heat from dry wear has the potential to lower wear resistance. It may soften structures that have been hardened, bring about phase transitions that make them more brittle and hard, reduce mechanical characteristics, and speed up corrosion reactions.

3. Welding

Welding is thought to be the main source of metallic material friction. The forces of cohesion between atoms of the same metal or metals with comparable crystal structures are quite strong. Metal interaction causes two clean surfaces of the same metal to join when they come into contact. High temperatures that soften metals make plastic deformation easier and make welding easier. Complete stopping may result from seizing. The extrapolation may result in scoring, galling, and excessive local wear. The risk of seizing can be reduced using a variety of techniques. One is to apply thin, rigid surfacing material layers. Using at least one metal that produces a thin, firmly adhering oxide, sulfide, or phosphide layer is generally beneficial. Aluminum oxide works wonders to stop welding. Seizures brought on by close contact caused by plastic deformation can be reduced using materials with a high elastic limit.

4. Impact

Since the rapidly imposed force may result in plastic flow and shape changes, the impact plays a role in wear. A properly designed surface should have a surface compressive yield strength greater than the impact's compressive stress.

5. Fatigue

Since fatigue failure degrades with time through use, it is discussed as part of wear. Increased fatigue strength will result from a proper design concentrating at notches and sharp angles to eliminate stress. Since tensile stress is always the cause of fatigue, residual compressive stress at the surface will prevent fatigue failure. Carburizing, for example, creates residual compressive stress during case hardening.

Seizing

It stops a moving point by a mating surface due to excessive friction caused by galling.

Scoring

Marring or scratching of any formed part by a metal pickup on the punch or die.

Protection against wear

Various technologies for providing surface protection to wear are as follows:

1. Electroplating
2. Anodizing
3. Diffusion
4. Metal Spraying
5. Hard facing
6. Selective Heat Treatment.

1. Electroplating

The wear resistance of a metal part can be improved by electroplating a harder metal on its surface. The metals most often plated on base materials are chromium, nickel and rhodium. Indium plating has been used to reduce the wear of lead bearings. Two types of chromium plating used industrially are known 1. Hard Chromium and 2. Porous Chromium. The hard chromium plate is the same as that used for decorative purposes but thicker. A porous chromium plate has carefully controlled pits or channels to hold lubricants on its surface. Another factor contributing to the reduction of wear is the low coefficient of friction of chromium plate. Now galling is another useful property of chromium plate. The high corrosion resistance of chromium helps in reducing wear under corrosive conditions.

2. Anodizing

The formation of an oxide coating by anodizing may be used to improve the wear resistance of contained metals. The anodizing process is usually applied to aluminum, magnesium, zinc and thin alloys. The work is the anode in anodizing, and oxide layers are built on the base metal. Since the newest oxide layer always forms next to the base

metal, for the process to continue, the previously developed oxide layers must be porous enough to allow the oxygen ions to pass through them. Anodizing aluminum is simply a method of building up a much thicker oxide coating that may be exposed to air. Anodizing zinc produces a coating with greater resistance to wear of the chromate film. The production of a hard, wear-resistant surface by anodizing has greatly extended the uses of magnesium and its alloys. Flash anodic coatings are often used as a base for print adherence.

3. Diffusion

Several processes improve wear resistance by diffusion some elements into the surface layers. There are:

1. Carburizing
2. Cyaniding
3. Carbonitriding
4. Chromizing
5. Siliconizing.

4. Metal Spraying

Metal or flame spraying has been used for years in production salvage to build up undersized dimensions and repair worn surfaces. Several methods can apply sprayed coatings. 1. Metallizing or flame plating is used to deposit Wc and aluminum oxide; 2. Plasma is spraying, which can deposit almost all inorganic materials. Metallizing is usually done by automatically feeding a metal wire at a controlled rate of speed through the metalizing tool or “gun”. Air, oxygen, and combustible gas are supplied to the gun by means of hoses and form a high-temperature, high-velocity flame around the wire tip. The wire tip is continuously melted off, and the liquid-metal particles are directed at the work by the high-velocity flame. Plasma is a luminous stream of ionized gas produced by passing a gas through an electric arc. Temperatures up to

30,000 °F are economically obtainable; thus, plasma flame permits the deposition of the highest melting metals. An additional advantage of the plasma process is that oxygen and combustion gas and their combustion products are absent from the gas stream.

5. Hard Facing

The production of a hard, wear-resistant surface later on metals by welding is known as Hard Facing. This method is relatively easy to apply, requiring only the hard-facing alloys in welding rods and an oxyacetylene flame or electric arc. The advantages of hard facing are that 1. It may be applied to localized areas subjected to wear 2. Hard wear-resistant compounds are available 3. It provides effective use of expensive alloys and protection in depth.

6. Selective Heat Treatment

The methods used for selective heat treatment are induction hardening and flame hardening. These are essentially shallow—hardening methods to produce a hardened case and relatively tough core.

Coring

A variable composition between the center and surface of a structural unit resulting from non-equilibrium growth occurs over temperatures.

Footnotes

¹ Chapter 8 is written based on the references J. P. Schaffer, A. Saxena, S. D. Antolovich, T. H. Sanders, and Steven B. Warner, 1999, “The Science and Design of Engineering Materials”, WBC/McGraw-Hill, USA, A. S. Khanna, 2002, “Introduction to High Temperature Oxidation and Corrosion”, ASM International, USA, Mars. G. Fontana, 1987, “Corrosion Engineering”, McGraw-Hill, 3 Ed, Singapore, Sydney H. Avner, 1997, “Introduction to Physical Metallurgy”, Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, “Foundations of Materials Science and Engineering”, 2004, McGraw-Hill, 3 Ed, New York, USA and William D. Callister Jr. & David G. Rethwisch, 2009, “Materials Science and Engineering: An Introduction”, 8th ed. John Wiley and Sons. NJ, USA.

9. Corrosion Engineering and Biomaterial Corrosion

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

9.1 Explain Various Aspects of Corrosion Engineering in Common Biomaterials i.e. Metallic Biomaterials¹

Corrosion

A metal begins to deteriorate through chemical or electrochemical reactions with its surroundings at the surface.

In certain cases, the corrosion products take the form of a thin, adhering coating that tarnishes or colors the metal and may deter further corrosive action. Other times, anti-corrosion compounds are thick and porous and provide little protection.

Corrosion is mostly brought on by the instability of metals in this fine condition. Corrosion usually causes the metals to return to their original conditions.

Electrolyte

Any ion-containing solution is an electrolyte. The electrolyte might be any concentration of pure water, salt water, acid, or alkaline solutions.

Cathodic Polarization

The process is slowed down as hydrogen coating builds up on the metal. This is known as cathodic polarization.

Electromotive-Force Series

The standard electromotive-force series indicates which metals may be anodic compared with hydrogen. Compared to the metals at the bottom of the list, the more active metals at the top have a stronger tendency to dissolve. In the solution, a metal higher in the series will push out a metal lower.

Galvanic Series

Only metals can be used in the electromotive series under the conditions that led to its innovation. Specific salt concentrations of the same metal under study were confirmed by the electrolytes.

An analogous galvanic series, based on knowledge of metal combinations in various environments, is used in place of the electromotive series. Such a series is provided in for various metals and alloys in fast-moving seawater. The metal closest to the top of any pair will be anodic and corrode, while the metal closest to the bottom will be cathodic and benefit from some galvanic safeguard. A metal linked with another metal near it on a thin list corrodes more slowly than one coupled with one below it.

Factor Influencing Corrosion

The variation in the electrical potential of dissimilar metals when linked and immersed in an electrolyte is one of the most fundamental elements determining corrosion. Because of the chemical properties of the anodic and cathodic zones, this potential exists. The relative concentrations of both ions in the reaction significantly impact electrical potential. The potential decreases as the metallic-ion concentration increases compared to the reducible ion concentration. Complete insulation and the cessation of corrosion occur when the metallic ion is eliminated by forming an insoluble compound that precipitates on the anode, sticks, and is impenetrable to the corroding solution. These kinds of oxide coatings give aluminium and chromium their outstanding corrosion resistance. When the part is exposed to alternate periods of immersion and drying, a porous oxide or metallic layer worsens corrosion.

Dissolved oxygen has two different effects on corrosion rates: first, it contributes to the creation of oxides, and second, it functions as a cathodic depolarizer. Corrosion will worsen if the oxide production removes the metal's metallic ions. Corrosion will accelerate if oxygen serves to remove hydrogen from the area surrounding the cathode. By bringing a new corroding solution into contact with the metal, agitation accelerates corrosion. Local action refers to variations in potential from one location to another on a single metal surface. They could be brought on by surface contaminants, variations in surface morphology, or environmental factors. Corrosion is brought on by localized environmental change. The corrosion rate may be significantly impacted by additional variables such as the presence of other ions in the solution, the solution's temperature, and stray elastic currents.

Uniform Corrosion

Uniform corrosion is when a metal's entire surface is equally corroded. Metals are used to measure this type because they are rarely so homogeneous that the surface will corrode uniformly.

Pitting Corrosion

Pitting corrosion, caused by inclusions, coring, and distorted zones in the metal is an example of non-uniform corrosion. These inhomogeneities allow variations at specific locations to result in deep, isolated holes. When the protective layer or film ruptures, the base metal begins to pit.

Cavitation

Rapid and intense pressure changes cause countless tiny voids or cavities to form and instantly collapse within a liquid.

Cavitation Corrosion

Cavities and bubbles within a liquid collapse, which results in cavitation corrosion. When a surface and a liquid vibrate so that the surface receives repeated loads and experiences regular bubble formation and collapse, extremely high stresses are generated. High-stress impacts from these collapses gradually remove material from the surface, forming deep pits, depressions, and pockmarks. This type of corrosion may be reduced or even prevented by using a more resistant material or a protective coating.

Crevice Corrosion

A general term for the faster attack at the junction of two metals subjected to a corrosive environment is crevice corrosion. Experience has taught us that crevices that retain solutions and take longer to dry out are more likely to experience corrosion. Even when completely submerged, corrosion can still happen in crevices. Due to a difference in oxygen concentration, the attack may accelerate. The outside joint is comparatively anodic and has relatively easy access to oxygen. An area with low oxygen concentration and an increased electrical potential is created by the deposit of insoluble corrosion product that forms around the anodic core as it tends to more completely exclude oxygen. A pit develops in the middle if the action continues. Where there is a lack of oxygen, corrosion always takes place.

Fretting Corrosion

Fretting corrosion is a frequent surface deterioration brought on by vibration, striking, or rubbing at the interface of two closely spaced, heavily loaded surfaces. Relatively light particles weld together when the adhesive force holds two components together. In the joint, debris or powder is formed due to chemical reactions between the welded particles and the atmosphere as they move very slightly.

Intergranular Corrosion

When there is a potential difference between the grain boundaries and the rest of the alloy, intergranular corrosion is another illustration of non-uniform corrosion, when a phase separates from a solid solution, this type of corrosion typically results. The material near the grain boundary becomes depleted of the dissolved element, producing a difference in potential, as precipitation typically occurs more quickly there. It will dissolve predominantly along the grain boundary. Visual examination of the component is frequently insufficient to determine the extent of the damage, and in the majority of cases, there has been a noticeable loss in mechanical characteristics.

Stress Corrosion Cracking

The combined effects of stress, either exterior (applied load) or interior (residual), and corrosion, referring to the corrosion environment on metal, are known as stress corrosion cracking—a metal's exposure to stress corrosion. Stress corrosion cracking is distinguished by a highly localized attack resulting from uniform corrosion that is very low or nonexistent overall. Stress causes strains, which lead to concentrated areas of increased energy. Fissures form when these zones become so chemically active that they are drawn to even a mildly corrosive environment. The fissures create a crack when under stress, raising the stress level in the body.

Stress Corrosion

When metals are under excessive external or internal stress due to cold working and stress corrosion cracking, stress corrosion speeds up corrosion in some environments. Transgranular, intergranular, or a combination of the two are possible cracks. By using protective coatings and keeping zinc contact in the case of brasses below 15%, it is possible to reduce the risk of

cracking and prevent residual stresses. Brasses with 20% to 40% zinc content are extremely vulnerable to attack.

Preferential Corrosion

One of the elements that could even happen in single-phase solid solution alloys is preferential corrosion. An illustration of this type of corrosion is dezincification in brass.

Galvanic Corrosion

At the point where two metals come into contact with a corrosive medium, galvanic corrosion takes place.

Liquid Metal Corrosion

Liquid metals like bismuth and sodium are employed as heat-transfer mediums in specific nuclear reactors to generate atomic power. The route of the liquid metal is a closed loop, with one leg in the reactor core at a high temperature and the other leg in the heat exchanger at a lower temperature. The temperature typically causes an increase in a solid's solubility in a liquid. Due to the lower solubility limit in the cooler leg, the solid has the propensity to dissolve up to its solubility limit in the high-temperature leg and then be deposited. The cold leg becomes plugged with the deposited corrosion products as the hot leg continues to corrode. Liquid metal inhibitors are the best way to stop this kind of corrosion. In liquid bismuth, zirconium has been used as an efficient inhibitor.

Methods for Combating Corrosion

By choosing the proper structure or surface protection for a given material, corrosion is prevented industrially using various techniques. The crucial ones are:

1. Use of high-purity metals
2. Use of alloy additions
3. Use of special heat treatments
4. Proper design

5. Cathodic protection
6. Use of inhibitors
7. Surface Coatings.

Parkerizing (Bonderizing or Phosphating)

Parkerizing is the corrosion method protecting ferrous alloy by forming a phosphate film.

Anodizing

Formation of thick oxide film on aluminum and magnesium.

Galvanizing

Zinc coating is called galvanizing.

Metallic Coating Methods

1. Metallizing
2. Hot dipping
3. Electroplating
4. Diffusion
5. Cladding.

Colorizing

Colorizing is the term used to describe the diffusion-based alloying of steel and aluminum. Highly resistant to oxidation and corrosion by hot gases, especially sulfurous gases, is colorized steel.

Sherardizing

Sherardizing is the term for zinc impregnation or vapor galvanizing. Sherardizing is primarily used on small steel components.

Cladding

Cladding is a technique for making the coating a permanent part of the material. You can do this by casting or hot working. The best conditions for casting are when the melting points of the base material and the cladding material differ significantly. The method for cladding that is more frequently used is hot rolling. An ingot of the base material is secured with slabs or sheets of the cladding material. The straps are taken off after heating to rolling temperature, and the entire assembly is rolled; the heat and pressure of rolling weld the two materials together. The base material that makes up the core may also make up the cladding. Al alloys that have been covered in pure aluminum to increase corrosion resistance are referred to as Alclad. Ni, Ni–Cr, or Ni-Cu alloys can be used to coat steel.

Surface Cleaning Methods

Surface cleaning involves the removal of unwanted material from the part's surface. There are 2 methods:

1. Mechanical Process

2. Chemical Process

3. Ultrasonic Cleaning

1. Mechanical Process

- Wire Brushing
- Tumbling
- Barrel and Vibrating Finishing
- Jet blast cleaning

2. Chemical Process

- Organic Solvent Cleaning
- Alkaline surfaces cleaning
- Pickling.

Wire Brushing

Surface cleaning removes contaminants such as surface scale and rust using a stiff wire brush. In most cases, it is the preliminary steps to subsequent operations; the most common is painting. Power-driven rotary brushes are more suitable than hand brushes for longer jobs.

Tumbling

Tumbling is another coarse cleaning process used to clean and deburr (remove rough edges). This simple process involves placing the casting to be cleaned inside a circular steel drum which is slowly rotated at typically 10–15 rpm. This rotary action results in the castings randomly hitting one another sufficiently hard to remove unwanted sharp edges. Some tumblers include loose material such as sand, granite chips or stones with the castings to enhance the cleaning process.

Barrel and Vibratory Finishing

Barrel finishing may be considered a refined tumbling form, although it also smooths and cleans surfaces. This is because abrasive particles in barrel finishing replace the non-abrasive material used in tumbling.

Artificial abrasives are normally used as their size and texture are easily controlled. Vibratory motion has taken over from true rotary motion in recent years. It is much more labor-intensive to load and unload barrel-type machines than the easily mechanized rotary vibration machines.

Furthermore, vibration frequency can be readily controlled to ensure a more precise and constant process than is possible with rotary barrel finishers.

Jet Blast Cleaning

One method of avoiding the physical impact between components in tumbling and barrel finishing is to strike the surface to be cleaned with a suitable fluid, the most commonly used being compressed air containing either steel shot or coarse sand. It is usually carried out in an enclosed cabinet to isolate the cleaning operation from the surrounding environment. The component to be cleaned is loaded into the working area of the jet blaster cabinet, and the fluid stream is directed either normally at the dirty surfaces or, less commonly, the workpiece is moved around under one or more fixed jets. Manual manipulation of jet work or component is carried out through a rubber glove box. The compressed air is typically used in the jet

blasting at a pressure of up to 6 bar. Much lower pressures are used for non-ferrous parts.

Organic Solvent Cleaning

Oils and greases are the commonest corrosion inhibitors used by industry. Still, when the parts protected by these substances are required for use, it is usually necessary to remove such protective coatings. Organic solvents are used for this degreasing activity. They are normally applied by either component immersion, spraying or vapour condensation, the precise method depending upon the size and the shape of the parts involved. Application by immersion or spraying is self-explanatory.

Alkaline Surface Cleaning

Organic solvents are an effective cleaning agent if the surface contaminants are organic solvent-soluble, but alkaline solutions are normally used if they are not. Furthermore, adding a water-soluble detergent to alkali creates a versatile cleaning medium that removes organic and most other forms of surface contamination. This explains why alkali-based cleaning is the most popular chemical cleaning process. Alkaline solutions can be applied to the work surfaces by immersion or spraying and are used as active agents in stream cleaning when the parts to be cleaned are too large to be dipped. To ensure that all traces of alkaline solutions are removed after cleaning, it is essential to rinse components thoroughly with water. Certain non-ferrous metals such as Al, Zn, tin and brass should not be alkali cleaned,

Pickling

Pickling may be defined as a process that removes the oxide layer from metal using acids and may or may not result in the erosion of the base metal. Thus, pickling is more a chemical descaling process than a surface cleaning one; it will be partially ineffective if, before pickling, the component's surface is not properly degreased. Its principal uses are in removing mill scale from hot rolled steel and removal of surface scale formed during certain types of the heat treatment process. It is also used for removing weld scale and heat discoloration from sheet metal fabrications. It is essential that over-pickling does not occur (leaving the component too long in pickling bath), as this results in surface pitting and hydrogen embrittlement problems in the case of steels. After pickling air, traces of

acid must be removed, normally achieved by dipping in an alkaline solution followed by a thoroughly clean water rinse.

Ultrasonic Cleaning

Suppose a low-viscosity liquid such as water is subjected to high-frequency (25–40 kHz) ultrasonic wave energy, or ultrasound as it is called, and intense cavitation is generated within the fluid. Cavitation is the generation and growth of vast quantities of gaseous bubbles within the fluid, which, upon reaching a certain size, typically 0.15 mm in diameter, implode (collapse inwards). As each bubble collapses, a microscopic inward-moving jet of fluid is created at an astonishing 250 mph, and it is this jet that blasts away contamination from the dirty surface. The sustained generation, growth and implosion of a huge number of bubbles throughout the ultrasonic bath and on all surfaces of the submerged component to be cleaned is referred to as the cavitation effect.

Surface Smoothing Processes

1. Hand Grinding
2. Belt Sanding
3. Polishing and Buffing
4. Electropolishing.

Hand Grinding

This is often erroneously classed as a cleaning process despite significant metal removal usually involved. It is more of a fettling/deburring/smoothing activity. Many surfaces need dressing or smoothing, an excellent example being weld dressing. Because the abrasive head is mounted in a hand-held portable grinder, the method offers great flexibility but is labour intensive.

Belt Sanding

Like hand grinding, this is also an abrasive process, the principle difference being that instead of the abrasive being presented to the workpiece in the

form of a rotating wheel or disk, the abrasive grits are glued to one side of a flat strip of flexible backing material (like sandpaper and emery paper). A suitable length of this abrasive strip is made up to form an endless loop, which is then slipped over the drive rollers of the belt sander.

Polishing

Occasionally it is necessary to enhance the appearance of an already clean and smooth surface still further by polishing. Polishing is done by hand-rubbing the work surface in a rotary or reciprocating motion while using a fine abrasive applied to a smooth, lint-free cloth. The workpiece can also be passively polished over the surface of a cloth polishing wheel that has been charged with abrasive until the desired surface is obtained.

Buffing

A finer abrasive, such as a jewelry range, is used for buffing as an extension of polishing. (Fe_2O_3) It is used when an extremely smooth surface finish is needed after polishing. It is possible to achieve mirror finishes, but polishing and buffing are labor-intensive, costly processes that should only be used when necessary for technical or economic purposes.

Electropolishing

Electropolishing is the reverse of electroplating in that a very thin layer (up to 40 pieces) of the component's surface is stripped away by deplating. This is achieved by reversing the polarity of a normal electroplating cell. The component is made of the anode (+) and placed adjacent to carefully designed and shaped cathode (–) plates. Both are immersed in a tank with a suitable electrolyte, such as phosphoric acid. When a high anodic current is applied, the surface layer of the workpiece migrates towards the cathode plates. Fortunately, this depleting action is not completely uniform across the whole jole profile, there being a preferential dissolving of the peaks of the surface profile. This helps to produce a smooth, bright finish.

Electroplating is mainly a finishing operation for machined surfaces. It is particularly suited to awkward shapes that do not lend themselves to polishing or buffing.

Footnotes

1 Chapter 9 is written based on the references A. S. Khanna, 2002, “Introduction to High Temperature Oxidation and Corrosion”, ASM International, USA, Neil Birks, Gerald H. Meier and Frederick S. Pettit, 2012, “Introduction to the High Temperature Oxidation of Metals”, Cambridge University Press, UK, Mars. G. Fontana, 1987, “Corrosion Engineering”, McGraw-Hill, 3 Ed, Singapore, Sydney H. Avner, 1997, “Introduction to Physical Metallurgy”, Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, “Foundations of Materials Science and Engineering”, 2004, McGraw-Hill, 3 Ed, New York, USA and William D. Callister Jr. & David G. Rethwisch, 2009 , “Materials Science and Engineering: An Introduction”, 8th ed. John Wiley and Sons. NJ, USA.

10. Heat Treatment

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

10.1 Describe Various Heat Treatment Aspects for a Common Biomaterial¹

Cold Work

The plastic deformation of metal under the action of applied forces is of great importance in the fabrication of metals to any desired shape. When it is carried out at a temperature, it is called the cold work of metals.

Hot-working

When the plastic deformation of metal is carried out at temperatures above the recrystallization temperature, no appreciable changes in mechanical properties occur. The process is called hot working. One of the primary goals of hot working is to produce a fine-grained product. Although there is no appreciable change in the mechanical properties, hot working effects contain other properties of metals. Density increases since many pores and cavities in the cast metal disappear during hot working.

Effect of Cold Working on Properties

When the plastic deformation of a material is complete and the grains are distorted, the material is said to have undergone cold working. Plastic deformation or cold working impacts all lattice-dependent properties of metals. While ductility, as measured by the elongation percentage, declines, tensile strength, yield strength, and hardness increase. Although both strength and hardness boost, the rates of change differ. It is crucial to keep in mind that the strength and hardness of the material will increase whenever the lattice structure is deformed, whether as a result of plastic deformation, heat treatment, or alloying.

Annealing

A limited quantity of energy used to cold-work the metal was stored in the crystal structure as internal energy associated with the lattice defects produced by the deformation, even though most of the energy was lost as heat during the process. The material retains the cold-work energy that was put into it in that fraction, typically between 1 and 10% of the energy used to create the cold-work state. The transformation of the distorted cold-worked lattice structure back to a strain-free one through heat is known as

full annealing. This entire procedure is carried out in the solid state, and the furnace's optimal temperature is slowly lowered. Recovering, recrystallization, and grain growth are the three stages that can be separated from the annealing process.

The annealing process softens metals, resulting in desired modifications to other characteristics or microstructures. Annealing is done for various reasons, such as to increase dimensional stability, facilitate hard work, improve mechanical or electrical characteristics, and improve workability. When the only goal is stress relief, the procedure is known as stress-relief annealing or stress-relieving annealing. Final annealing, full annealing, recrystallization, and stress-relief annealing are specific process names that are used commercially. Some of them are “In-shop” terms without clear definitions.

Recovery

Since this process is primarily low-temperature, the resulting property changes do not significantly alter the microstructure. The main benefit of recovery appears to be the reduced internal tension brought on by cold working. All the elastic deformation is still present after the load that caused plastic deformation in a polycrystalline material is removed. Most internal stress is relieved as some of these elastically displaced atoms spring back as the temperature rises. During the recovery stage, there was a marginal increase in hardness, strength, and electrical conductivity. The main use of heating in the recovery range is in stress-relieving cold-worked alloys to prevent stress-corrosion cracking or minimize the distortion brought on by residual stresses because the metal's mechanical properties remain unchanged. Stress-relief annealing is the name given to this low-temperature treatment in the recovery range by industry.

Recrystallization

Insignificant new crystals appear in the microstructure as the recovery range's upper temperature is reached. These innovative crystals are not elongated but rather roughly uniform in size and share the same composition and lattice structure as the original underinformed grains (equiaxed). The most severely deformed areas of the grain, typically the grain boundaries and slip planes, are where the new crystals typically form. The collection of atoms in a nucleus is where new grains are created.

Incorporating strain-free grains and allowing their growing nuclei to absorb the entire cold-worked material leads to recrystallization. Recrystallization's exact mechanism is still not fully understood. However, Fig. 10.1 depicts a condensed analogy.

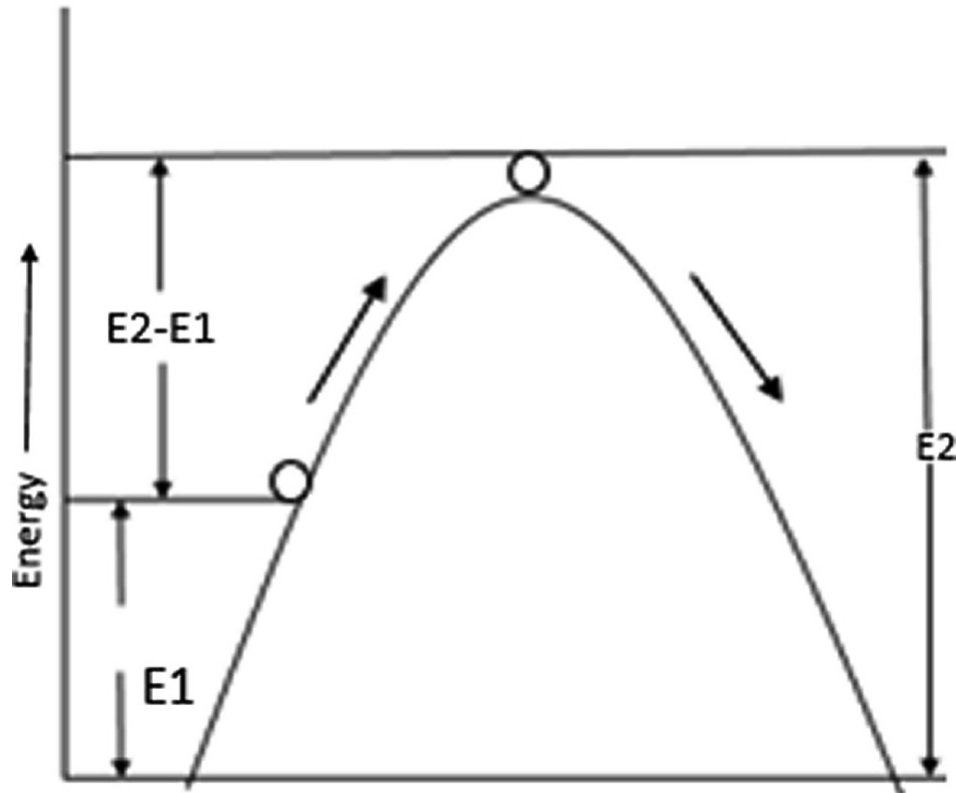


Fig. 10.1 A simplified analogy of Recrystallization (Avner, 1997)

Imagine that certain atoms were also pressured up an energy hill to a value E_1 higher than the atoms' internal energy in the undisturbed lattice at grain boundaries or slip planes. E_2 is the amount of energy needed to break through the rigidity of the distorted lattice. The atoms cannot rise the hill to the energy of the strain-free crystal using the same route; rather, they must rise to the top, from which they can easily come down. Heat is the source of this energy difference ($E_2 - E_1$). When the temperature reaches E_2 , these localized areas lose some of their energy as heat from recrystallization and the nuclei of strain-free grains. A portion of this recrystallization heat is taken up by the area, giving the nearby atoms the energy they need to overcome the rigidity of the distorted lattice and be drawn into the lattice structure of the strain-free grains, causing grain growth. The quantity of

prior deformation significantly impacts the number and energy of these high-energy points, with quantity increasing with increasing deformation.

Recrystallization Temperature

The term “recrystallization temperature” refers to the approximate temperature at which a highly cold-worked material completely recrystallizes in one hour rather than the actual temperature below which recrystallization will not occur. Remember that alloys and impure metals have higher crystallization temperatures than pure metals. Recrystallization temperatures for zinc, tin, and lead are below room temperature. These metals spontaneously recrystallize, forming a strain-free lattice structure, making it hard to work them at room temperature. The recrystallization temperature falls as the annealing time increases. Compared to time variations at a constant temperature, the recrystallization process is much more sensitive to temperature changes. Before any change in grain size occurs, a deformation of about 7% is necessary. Critical deformation is the term used for this. At degrees of deformation smaller than this, the number of recrystallization nuclei becomes very small. i.e., a certain minimum amount of cold-working (7%) is necessary for recrystallization.

Scale

Scale is the name given to the distinctive dark oxide coating. This scale indicates the difficulty of machining or forming operations.

Grain Growth

Small grains have more free energy, while large grains have less. This is connected to the lessening of the grain boundary. Consequently, under ideal circumstances, a single crystal of metal would have the lowest energy. This is the fuel that propels the growth of grains. The rigidity of the lattice is in opposition to this freedom. The rigidity of the lattice reduces as the temperature rises and the grain growth rate accelerates. There is the largest grain size at which these two aspects are in equilibrium at any given temperature. Consequently, trying to hold a specimen in the grain-growth region for a long time should theoretically allow for the growth of very large grains. The specimen was kept at a temperature just below this alloy's melting point to produce large grain.

Grain Size

Given that annealing involves nucleation and grain development, fine-grained material will be produced if conditions favor rapid nucleation and growth. Those that favor rapid growth and slow nucleation will produce coarse-grained material. The following variables influence the final recrystallization grain size:

1. Degree of Prior Deformation: They favor nucleation, enhance the amount of earlier deformation, and reduce the size of the finished grain. Upon annealing, the grains will be enormous at the critical deformation. Assume that the critical amount of deformation is carefully controlled. The degree of deformation will then increase, and subsequent annealing will produce very large grains or single crystals. This causes recrystallization from more grains, which results in steadily smaller grain sizes.
2. Time at temperature: We are keeping an object at a temperature higher than the recrystallization temperature encourages grain growth and grows the final grain size.
3. Annealing temperature: The final grain size will be finer the lower the temperature is above the recrystallization temperature.
4. Heating time: The final grain size is finer the faster it is heated to the annealing temperature. Few nuclei will form during slow heating, promoting coarse grain and grain growth.
5. Insoluble temperature: The final grain size will be finer the more insoluble impurities there are and the more evenly distributed they are. They serve as barriers to grain growth in addition to increasing nucleation. The final grain size is barely impacted by the rate of cooling from the annealing temperature.

Effect of properties

Full annealing is primarily a softening procedure because it returns the material to a strain-free lattice structure. Hardness and strength are reduced while ductility is increased during annealing.

Spheroidizing

Spheroidizing annealing is a type of heat-treating that increases workability. In a ferric matrix, this process will result in a globular or spheroidal form of carbide. For this process, one of the following approaches could be employed.

1. Prolonged holding at a temperature just below the critical line.
2. Heating and cooling alternately between temperatures above and below the lower critical line.
3. Heating to a temperature above the lower critical line and then cooling very slowly in the furnace or holding at a temperature below the lower critical line.

Process Annealing

The steel is heated to a temperature between 1000 and 1250 degrees Fahrenheit (below the lower critical line) for this heat treatment, which is used in the sheet and wire industries. It is used after cold working and, through recrystallization, softens the steel for further processing. It resembles stress-relief annealing a lot.

Normalizing

A homogenizing or grain-refining process called normalizing aims to homogenize a part's composition uniformly. Steel is normalized by heating it to a temperature about 100 °F (55 °C) above the upper-critical-temperature (A_3 or A_{cm}) line, then cooling it to room temperature in still air. For normalizing to be the final heat treatment for some applications, normalizing must produce steel that is harder and stronger than full annealing.

Hardening

Hardening is the process of increasing hardness through appropriate treatment, typically heating and cooling. The hardening process involves heating to the hardening temperature, maintaining the temperature, and then rapidly cooling, like quenching in water. If the cooling rate exceeds the upper critical cooling rate, it is said to be cooling rapidly. When appropriate, the more precise terms for hardening would be:

1. Age hardening,
2. Case hardening,
3. Flame hardening
4. Induction hardening
5. Precipitation hardening
6. Quench hardening

Martensite is a supersaturated interstitial solid solution of carbon trapped in a Body-Centered-Tetragonal structure.

The carbon atoms in the austenite structure can diffuse out under slow cooling rates. After that, the iron atom shifts a little to become BCC. This γ to α transplanted is a time-dependent procedure that entails both nucleation and growth. This γ to α transplanted takes place through a process of nucleation and growth and is time-dependent. The structure cannot become BCC while the carbon is trapped in the solution, though, because an increase in cooling rate or rapid cooling does not allow enough time for the carbon to diffuse out of the solution. Therefore, a different type of phase transformed and the transformed phase depend solely on temperature, not time. The final structure is known as martensite.

Martensitic Transformation

A reaction in some metals on cooling forms an acicular structure named martensite.

Bainite

Eutectoid of α -Ferrite and cementite. The α -Ferrite has either a feathery appearance or occurs as plates. Carbide particles lie between the α -Ferrite regions.

It is a byproduct of austenite's decomposition, made up of ferrite and carbide. It typically forms at temperatures greater than those where martensite regions include cooling and lower than very fine pearlite forms.

Bainite forms when austenite is quenched to a temperature below the pearlite region but above the martensite start temperature.

Aging

A change in properties of metal or alloy generally occurs slowly at room temperature and rapidly at high temperature after heat treatment or cold-working or hot-working. Phase change seems to be what causes the change in characteristics; the chemical makeup of the metal or alloy is never involved. Natural aging alloys are those in which precipitation requires

room temperature to reach maximum strength. Artificial-aging alloys are those that have to be heated up again to reach their maximum strength.

Age Hardening or Precipitation Hardening 1

Hardening by aging, usually after rapid cooling or cold working.

Cold working or heat treatment are the only two main ways to increase an alloy's strength and hardness; age-hardening is the most crucial heat-treating process for non-ferrous alloys.

Case Hardening or Surface Hardening

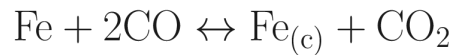
In many commercial processes, the case, which has a hard wear-resistance surface, and the core, which has a relatively soft, tough interior, are both necessary. The top 5 case hardening techniques are as follows:

1. Carburizing
2. Nitriding
3. Carbonitriding or cyaniding
4. Flame Hardening
5. Induction Hardening.

1. Carburizing

Carburizing is introducing carbon through absorption and diffusion into solid ferrous alloys by heating to a temperature higher than the alloy's upper transformation temperature. Low-carbon steel, typically with a carbon content of 0.2% or less, is exposed to a carbon monoxide environment. The temperature used for carburizing is generally in the range of 900–1040 °C (1150–1920 °F). It is possible to harden the surface layers to a high degree either by quenching (drastic cooling) from the carburizing temperature or by cooling to room temperature, austenitizing, and quenching. The heating process creates a carbon gradient extending inward from the surface. The carburizing equation ($\text{Fe} + 2\text{CO} \rightarrow \text{Fe}_{(\text{c})} + \text{CO}_2$) is reversible and may proceed to the left,

removing carbon from the surface layer if the steel is heated in an atmosphere containing CO₂. This is called decarburization.



Commercial carburizing may be accomplished by means of 1. Pack carburizing 2. Gas carburizing, and 3. Liquid carburizing.

2. **Nitriding**

The introduction of nitrogen into the surface layers of certain ferrous alloys by holding at a suitable temperature below the lower transformation temperature (A_{C1}) in contact with a nitrogen environment (such as ammonia, NH₃) is known as nitriding. Processing temperature is generally in the range of 525–565 °C (975–1050 °F), and the nascent N₂ may be generated by cracking anhydrous ammonia (NH₃) or from molten salts that contain cyanide. Quenching is not required.

3. **Carbonitriding or Cyaniding**

Carbonitriding is a case-hardening process in which a ferrous material (often a low-carbon grade of steel) is heated above the transformation temperature in a gaseous atmosphere of such composition to cause simultaneous absorption of carbon and nitrogen by the surface and by diffusion, creating a concentration gradient. The process is completed by cooling at a rate that produces the derived properties in the workpiece. Carbonitriding is most widely used for producing thin, hard, wear-resistant cases on numerous hardware items.

4. **Flame Hardening**

It's a shallow hardening method. Selected steel surface areas are heated into the austenite range and then quenched to form martensite. Therefore, it is necessary to start with steel capable of being hardened. Generally, this is in 0.3–0.6% carbon.

5. **Induction Hardening**

When a metal is placed in a rapidly varying magnetic field, currents induced in the metal cause heating, resulting in induction hardening. After the steel has been heated to the proper austenizing temperature and required depth, quenching is accomplished by introducing a water spray or other suitable fluid through the spaces between the inductor coil. The induction hardening process is also a shallow hardening method.

Tempering

Tempering is a heat-treatment process. A previously hardened or normalized steel is usually heated to a temperature below the lower critical temperature and cooled in air or at any suitable rate to decrease the hardness and increase the ductility and toughness. It is also used to relieve residual stresses due to quenching.

Martempering

Quenching an austenized ferrous alloy in a medium at a temperature in the upper part of the martensite range or slightly above that range and holding it before quenching in the medium until the temperature throughout the alloy is substantially uniform. The alloy is then allowed to cool through the martensite range. The concept is to delay cooling to minimize the distortion, cracking and residual stress. It is better to call this process “marquenching”.

Austempering

This is a special heat treatment process where austenite is transformed into bainite. Austenite is generally transformed into pearlite or martensite during conventional heat treatment processes involving continuous cooling.

Austempering consists of heating steel above the austenitizing temperature. It is then quenched in a bath maintained at a constant temperature above M_s point and within the bainitic range (200–400 °C, in general). The steel is quenched and maintained at a constant temperature in the bath until all the austenite is transformed into bainite. Since the process involves the transformation of austenite to bainite at a constant temperature, it is also known as isothermal quenching or isothermal hardening.

Austenitizing

Form austenite by heating a ferrous alloy above the transformation range.

Footnotes

¹ Chapter 10 is written based on the references J. P. Schaffer, A. Saxena, S. D. Antolovich, T. H. Sanders, and Steven B. Warner, 1999, “The Science and Design of Engineering Materials”, WBC/McGraw-Hill, USA, Sydney H. Avner, 1997, “Introduction to Physical Metallurgy”, Tata McGraw-Hill, 2 Ed, New York, USA, William F. Smith, “Foundations of Materials Science and Engineering”, 2004, McGraw-Hill, 3 Ed, New York, USA and William D. Callister Jr. & David G. Rethwisch, 2009, “Materials Science and Engineering: An Introduction”, 8th ed. John Wiley and Sons. NJ, USA.

11. Solution Chemistry and Chemical Reaction

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering, Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei Darussalam
- (2) Department of Mechanical Engineering, School of Computing, Engineering and Built Environment, Glasgow Caledonian University, Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia, Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering, Faculty of Mechanical Engineering, Universiti Teknologi Malaysia, Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

11.1 Chemistry of Solution

pH: The negative logarithm of the hydrogen ion solution concentration is pH.

$$\therefore p^H = -\log [H^+]$$

$$\therefore [H^+] = 10^{-p^H}$$

and

$$p^{OH} = -\log [OH^-]$$

$$\therefore [OH^-] = 10^{-p^{OH}}$$

also,

$$p^H = p^{OH} = 7 \text{ [} @298 \text{ K and neutral solution]}$$

and

$$p^H + p^{OH} = 14$$

@298 K in a neutral solution :

$$[H^+] = [OH^-] = 10^{-7} \text{ gm/dm}^3$$

$$\therefore p^H = p^{OH} = -\log 10^{-7} = 7$$

Buffer Solution

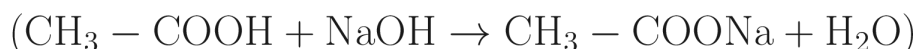
The solution in which the pH does not change after adding a limited amount of acid or base is called a buffer solution.

The process that protects against pH damage in a limited amount is called buffer reaction.

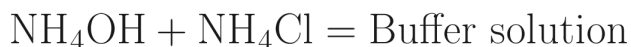
Usually, the buffer solution is prepared by mixing weak acid and the salt of the strong base of that weak acid. For example:



where CH_3COONa is the salt of



Sometimes weak base + its acid produce a base buffer solution. For example:



Calculation of pH of Buffer Solution

By using Henderson's equation:

$$\text{p}^{\text{H}} = \text{p}^{\text{K}_a} + \log \frac{[\text{Salt}]}{[\text{Acid}]}$$

where K_a = Dissociation Constant of acid

$$= \frac{[\text{H}^+] [\text{Salt}]}{[\text{Acid}]}$$

Acid–Base Indicator

By changing its color, the compound indicates a solution, whether an acid or base or neutral, or determines the reaction's endpoint, called an acid–base indicator.

Indicator	Acid-Base	
Phenolphthalein (Hln)	Colorless	Pink
Methyl orange	Red	Orange
Methyl red	Red	Yellow
Bromophenol	Yellow	Blue
Methyl yellow	Red	Yellow
Thymol blue	Red	Yellow

Dissolution

A solid, liquid, or gas becomes a solution when it dissolves in a solvent.

The collapse of the crystal lattice into individual ions, atoms, or molecules in solids and their transport into the solvent can be used to explain this.

pH

Equilibrium Constant (K_c)

If a reversible reaction is:

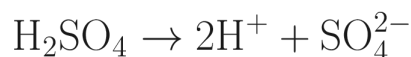


According to the law of mass action,

$$K_c = \frac{[L]^l \cdot [M]^m}{[A]^a \cdot [B]^b}$$
$$= \frac{\text{Molar concentration of Product}}{\text{Molar concentration of Reactant}}$$

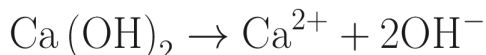
Acid (Arrhenius Theory)

The materials that molecules have hydrogen atoms and produce hydrogen ions (H^+) by dissociation in an aqueous solution are called acids. Such as:



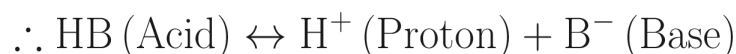
Base (Arrhenius Theory)

The hydroxide compounds that produce hydroxide ion (OH^-) dissociation in an aqueous solution are called bases. Such as:



Acid and Base (Bronsted-Lowry Theory)

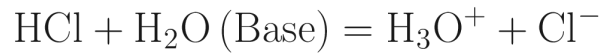
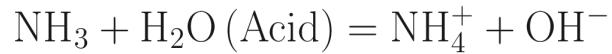
The materials that give proton (p^+) in a solution are called acid, which receives proton in a solution and is called the base. Such as:



Amphoteric Material

According to “the concept, a partionary material can act as an acid or base in different fields. This kind of material is called amphoteric material.

Example H₂O



Ionic Product of Water



∴ according to the law of mass action

$$K_c = \frac{[\text{OH}^-] [\text{H}^+]}{[\text{H}_2\text{O}]}$$

$$\rightarrow K_c [\text{H}_2\text{O}] = [\text{OH}^-] [\text{H}^+]$$

Since water is ionized, very little, i.e., [H₂O], is assumed to be constant.

$$\therefore K_c [\text{H}_2\text{O}] = K_w = \text{constant}$$

$$\therefore K_w = [\text{OH}^-] [\text{H}^+]$$

$$@298 \text{ K } (25^\circ \text{C}) ; K_w = 10^{-14}$$

$$\therefore K_w = [\text{OH}^-] [\text{H}^+] = 10^{-14} @ 298 \text{ K}$$

$$\text{If } [\text{H}^+] > [\text{OH}^-] = \text{Acidic}$$

$$\text{If } [\text{H}^+] < [\text{OH}^-] = \text{Base}$$

$$\text{If } [\text{H}^+] = [\text{OH}^-] = 10^{-7} = \text{neutral} = \text{Pure Water} @ \text{any temperature}$$

PVD

Physical mechanisms (evaporation or collision impact) cause source atoms to enter the gas phase during physical vapor deposition, which depends on solid or molten sources. Gaseous species are transported in environments with reduced pressure, where chemical reactions are typically absent. (“ ”)



CVD: Vapor $\rightarrow$ Solid reaction

Advantages

1. The deposition rate is higher than in CVD.
2. PVD process is a low deposition temperature compared to CVD.

Disadvantages

1. The diamond film quality of CVD is better than PVD.
2. Do not produce uniform coating around corners for microelectronics application compared to CVD.

Types

PVD

1. Evaporation
 - HF evaporation
 - Electron beam evaporation
2. Sputtering
 - “ ”
 - RF magnetron sputtering
 - DC magnetron sputtering
 - Ion Beam sputtering
 - Reactive sputtering
 - Ion assisted sputtering
 - High target utilization sputtering
 - High power impulse magnetron sputtering
 - Gas glow sputtering
3. Ion plating

- Electron beam ion plating
- Cathodic arc plating
- Anodic arc plating

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12. Basic Human Biology in Terms of Anatomy and Histology

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering, Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei Darussalam
- (2) Department of Mechanical Engineering, School of Computing, Engineering and Built Environment, Glasgow Caledonian University, Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia, Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering, Faculty of Mechanical Engineering, Universiti Teknologi Malaysia, Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

12.1 Describe A Common Musculoskeletal System From Biomaterials Application Aspects (Anatomy of Knee)¹

Articulations—In Anatomy, a common area is when two bones are attached for the motion of body parts. An articulation or joint is usually formed of fibrous connective tissue and cartilage.

Cartilage—Firm, rubbery tissue that cushions bones at joints.

Tendon—The tissue by which a muscle attaches to the bone. A tendon is somewhat flexible but fibrous and tough.

Bursae—A closed fluid-filled bag that provides a gliding surface to reduce friction between body tissues.

Ligament—A ligament is a tough band of connective tissue that connects various structures, such as bones.

Synarthrosis (Immovable joints)—The long edges are close together, and many interlocks. These extremely strong joints are located where movement between the bones must be prevented.

- **“Suture”**—(a “securing” together)—by dense connective tissue

Examples: the bones of the skull.

- **Gomphosis**—(a “bolting” together)—the fibrous connection

Examples: tooth-to-bone sockets.

- **Symphysis**—(together and cartilage)—a rigid cartilaginous connection bridge between two articulating bones

Examples: vertebral ribs and the sternum.

- **Synostosis**—(totally rigid and no movable joints)—between two separate bone fuse and boundary disappears.

Examples: metopic suture.

Amphiarthrosis (Little movable joints) permit more movement than synarthrosis but is stronger than a freely movable joint. Collagen fibers connect the articulating bones on cartilage.

- **Syndesmosis** (a band of ligaments)—bones are connected by a ligament

Example—(between tibia and fibula)

- **Symphysis** (symphyseal joint)—the articulating bones are separated by a wedge, pad, or fibrocartilage.

Example—Between the bodies of vertebrae. The connection between the two pelvic bones.

Diarthrosis (Freely Movable Joints)—Diarthrosis or synovial joints is surrounded by a fibrous articular capsule and a synovial membrane which consists of areolar tissue covered by an incomplete epithelial layer. This synovial membrane lines the walls of the articular cavity. The synovial fluid that fills the joint cavity originates in the areolar tissue of the synovial membrane.

Example: knee joints.

Synovial Fluid—Synovial fluid resembles industrial fluid but contains a high concentration of proteoglycans secreted by fibroblasts of the synovial membrane. A thick, viscous solution with the consistency of heavy molasses, the synovial fluid within a joint has 3 primary functions: lubrication, nutrient distribution, and shock absorption.

Fat Pad—Fat pads are localized adipose tissue masses covered by a synovial membrane layer. It protects articular cartilage and is not a packing material for the joint. It fills up the spaces of the cavity where bone moves.

Stress Shielding Effect—Reduction of bone density due to removing normal stress from the lower leg by the implant.

12.2 Name Various Types of Proteins and Describe Common Terminology of Basic Histology²

Proteins

Fibrous Proteins

1. Cytoskeletal Proteins

- Actin
- Arp 2/3
- Coronin
- Dystrophin
- Ftsz percentage
- Keratin
- Myosin
- Spectrin
- Tau
- Tubulin

2. Extracellular Matrix

- Collagen
- Elastin
- F-spondin
- Pikachurin.

Globular Protein

Plasma Protein

- Serum, Amyloid P component
- Serum
- Albumin
- Globulin
- Fibrinogen.

Coagulation Factors

- Component Proteins
- C1 inhibitors
- C3 convertase.
- Factor VIII
- Factor XIII
- Fibrin

- Protein C
- Protein S
- Protein Z
- Thrombin
- Von Willebrand Factor.

Hormones

1. Insulin
2. Epidermal Growth Factor
3. Insulin-like Factor
4. Oxytocin.

Receptor

1. G-Protein coupled receptor
2. Rhodopsin
3. Estrogen receptor.

Immune System

1. Immunoglobulin
2. Major histocompatibility antigen
3. T cell receptor

4. Ferritin

5. GroEL percentage.

Acute Phase Protein

Hemo Proteins

Cell Adhesion

1. Cadherin

2. Ependymin

3. Intergrin

4. NCAM

5. Selectin

6. ICAM-1.

Transport Proteins

1. CFTR

2. Glycophorin

3. Scrambles.

Enzymes

ICAM-3: Inter-cellular adhesion molecule in a protein.

Pathogen: A germ or organism such as a virus, bacteria, or fungi that causes disease in an animal host.

Necrosis: Premature death of the cell.

Metallosis: Toxicity or inflammation due to metallic wear debris in the soft tissue.

Calcification: The process of calcium salts build up in soft tissue, which causes it to harden.

Confluency: The number of cells in a cell culture dish or a flask refers to the cells' coverage of the dish or flask. Example: 100% confluency means the dish is completely covered by the cells, and there is no more place left for the cells to grow.

Arthroplasty: In orthopedic surgery, the arthritic or dysfunctional joint surface is replaced with an orthopedic prosthesis.

Blood: Blood is a special connective tissue consisting of cellular elements, plasma (fluid), metabolites and proteins.

Plasma: Plasma is a proteinaceous solution in which cells circulate and carries materials, metabolic, antibody, hormones.

Serum: Plasma-calcium.

Tissue is a cellular organizational level intermediate between cells and complete organisms.

Eukaryotic cells: The cells with a nucleus.

Prokaryotic cells: Which don't have a nucleus.

Type of Tissue:

1. Epithelial tissue
2. Connective Tissue

3. Muscle or Muscular Tissue

4. Nervous Tissue.

Endothelium Cells

The endothelium is the thin layer of cells that lines the interior surface of blood vessels.

1. **Epithelium**

Epithelium or epithelial tissue is one of four basic tissues. It consists of continuous sheets (layers) of cells that cover outer body surfaces (skin). It also lines internal cavities such as the digestive, respiratory, cardiovascular and genitourinary systems.

2. **Connective Tissue**

A major connective function provides form and support to the body and organs and connects and anchors other parts. It has three main components: 1. Cells, 2. Fiber, and 3. Extracellular matrix. It is also a medium for exchanging nutrients, oxygen gas, and waste products between other tissues, defense and protection, and storing fat (adipose tissue) for cushioning. Connective tissue makes tendons, cartilage, bone, blood, and adipose tissue.

3. **Muscle Tissue**

Muscle is a specialized tissue whose cells can contract (shorten) when stimulated and relax passively. Muscle cells derive their electricity from the arrangement of actin (thin) and myosin (thick) protein, “which can use energy to move relative to one another. They are classified as skeletal, cardiac and smooth muscles.

4. **Nervous Tissue**

Nervous tissue is the main component of the nervous system—the brain, spinal cord, and nerves that regulate and control body functions. Nervous tissue comprises two types of cells: 1. Nervous and 2. glial cells.

Fibroblasts

Fibroblasts are the main cell type of connective tissue. The extracellular matrix (ECM) synthesizes and secretes ground substances and connective tissue fibers, including collagen and elastic reticular fibers, in the extracellular matrix (ECM). These cells are inactive and immobile in mature connective tissue and are often called fibrocytes. After injury and wound repair, they rapidly increase and become active fibroblasts to synthesize new EC fibers and ground substances.

Adipose Tissue

Adipose tissue is a specialized “connective tissue that contains many adipocytes. It functions in insulation and padding and provides a ready fuel source for the metabolic process. Adipose tissue usually constitutes 15–20% body weight. It is highly labile tissue, specialized in synthesizing and storing lipids. Fat may be formed directly from carbohydrates in adipocytes.

Histocyte is a mononuclear phagocyte cell, which means monocytes and a tissue macrophage.

TNF- α : Tumor necrosis factor refer to a group of cytokines.

Apoptosis: Process of cell death.

Passage Number: The passage number is the number of tissues that the culture has been subcultured.

Generation Number: The generation number is the number of doublings the cell population has undergone.

Finite Cell Line: Cell lines with limited culture life spans are known as finite cell lines.

Collagen is a protein that produces mammals' flesh and connective tissues.

Osteoblasts: A mononucleate cell that is responsible for bone formation. The osteoblast is a specialized fibroblast, i.e., attached type cells. This is mainly composed of Type 1 collagen.

MTT assay: 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide, a yellow tetrazole, an indicator dye used to assess viability.

Saos-2: Sarcoma osteogenic is a cell from osteosarcoma of an 11-year-old Caucasian girl. It poses osteoblastic.

Carcinogen: A carcinogen is any substance or radiation that is an agent directly involved in causing cancer.

Mutagen: Mutagen is a physical or chemical agent that changes an organism's genetic material, normally DNA, and thus increases the frequency of mutations.

Genotoxicity: Genotoxicity test is defined as in vitro or in vivo tests that aim to detect compounds or elements that introduce genetic change, including DNA damage, gene mutation, chromosomal breakage, altered DNA repair capacity and cellular transformation. In other words, genotoxicity means a change in the morphology of a cell instead of cell death.

Orthodontics: The study and treatment of improper bites resulting from tooth irregularity, disproportionate jaw relationship, or both.

Endodontics: The study and treatment method that deals with pulp and the tissue surrounding the root of a tooth. For example, root canals.

Peri-Implantitis: A dental term used to describe the destructive inflammatory process affecting the soft and hard tissues surrounding dental implants.

Osseointegration: The term refers to the direct structural and functional connection between living bone and the surface of a load-bearing implant.

Mutagenicity: In generics, a mutagen is a physical or chemical agent that changes the genetic material, normally DNA and thus increases the mutation process.

Osteogenic: In laying down new bone material by cells called osteoblasts.

Peroxidation: It refers to the oxidative degradation of liquids.

Bioactivity: ADME → Absorption, distribution, metabolism and excretion, i.e., beneficial effects of the drug on living matter.

Footnotes

¹ Chapter 12 is written based on the reference W. K. Ovalle and P.C. Nahirny, “Netter’s Essential Histology”, 2008, Elsevier, USA, Elaine N. Marieb, “Essentials of Human Anatomy & Physiology”, 8th Ed, 2005, Pearson, USA and C. Starr and R. Taggart, “Cell Biology and Genetics”, Wadsworth Publishing, 1995, USA.

² Chapter 12 is written based on the reference W. K. Ovalle and P.C. Nahirny, “Netter’s Essential Histology”, 2008, Elsevier, USA, Elaine N. Marieb, “Essentials of Human Anatomy & Physiology”, 8th Ed, 2005, Pearson, USA and C. Starr and R. Taggart, “Cell Biology and Genetics”, Wadsworth Publishing, 1995, USA.

13. Biomaterials Cell Testing and Charactersitation

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ ,
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Facutly of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

13.1 Show an example of In-Vitro Testing through Human Cell

Cell Line

U937 cells (catalogue no. 85011440) (Human Caucasian histiocytic lymphoma) (available from ECACC, United Kingdom) derived from malignant cells of a pleural effusion of 37 year old Caucasian male with diffuse histiocytic lymphoma.

Cell Maintenance

U937 cells were cultured according to the protocol of Freshney (2005). The cells were grown in RPMI 1640 medium (cat. No. 11875, In vitrogen) with addition of 2 mM Glutamine and 10% Foetal Bovine Serum (FBS). The suspension cultures were maintained between 2 and 9×10^5 cells/ml; 5% CO₂; 37 °C. The cells reached confluence within 72 h.

Cell Cryopreservation

Cells at log phase can be frozen for storage. Cells were centrifuged before adding with freezing medium. The freezing medium consisted of 90% FBS and 10% DMSO. Normally, 1×10^6 cells/ml was used for cryopreservation in 1.2 ml cryogenic vial. The vial was brought down to freezing temperature using freezing container (Nalge Nunc). After approximately 24 h at -80 °C, the vial was transferred to liquid nitrogen tank for long storage (Freshney 2005).

Cell Recovery

Cryopreserved vial of cells was removed from the liquid nitrogen storage tank using proper protection. The cells were rapidly thawed by placing the vial in a 37 °C water bath for 1 min or until completely thawed. The cell suspension was quickly removed from the vial into the flask containing 15 ml pre-warmed growth medium. Cells were allowed in a 37 °C, 5% CO₂ humidified incubator. For best result, it is advisable not to disturb the culture for 24 h after inoculation revived.

U937 Cell Culture Protocol for Metal Ion Released Study

Three test cultures were prepared. Each test cultures was seeded with 2×10^5 cells/ml in 30 ml medium and cultured in 75 cm² flask for 30 days (37 °C, 5% CO₂). Titanium alloy and oxidized samples were immersed in T- flasks separately and then incubated in the 5% CO₂ humidified incubator at 37 °C.

Table 13.1 The summary of handling metal ion released experiment

Test culture	Medium + cells		
	Bare Metal (Control)	6 hours oxidized	12 hours oxidized
T-Flask	75 cm ²	75 cm ²	75 cm ²
Handling volume	30 ml	30 ml	30 ml
Legend	c	1	2

All the test cultures were incubated at 37 °C, 5% CO₂, for 30 days. Medium sampling was done on day 1 and 30. For sampling purpose, 2 ml medium were taken out. and then followed by spin down at 3300 rpm for 10 min. Supernatant were kept at –80 °C for further analysis. The supernatant was analyzed in ppb by inductively coupled plasma-mass spectrometry (ICP-MS, Perkin Almer ELAN/6100, Vernon Hills, Illinois USA). The dilution was prepared for 0.1 ml × 10 ml.

Reference

R. Ian Freshney, “Culture of Animal Cells”, John Wiley & Sons, 2005, ISBN: 9780471453291.

14. Biomaterials and Their Properties

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering,
Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei
Darussalam
- (2) Department of Mechanical Engineering, School of Computing,
Engineering and Built Environment, Glasgow Caledonian University,
Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia,
Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering,
Faculty of Mechanical Engineering, Universiti Teknologi Malaysia,
Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

14.1 Describe Properties of a very common biomaterial (Titanium)¹

Group → 4, Block → d, Atomic no. → 22

Transition Metal

1. Atomic weight → 47.90

2. Electronic structure → [Ar] 3d²4s²

3. Melting Point → 1677 °C

4. Boiling Point → 3277 °C

5. Transition Temperature ($\alpha \rightarrow \beta$) → 882.5 °C

6. Density (25 °C) → 4.5 g/cm³

7. CTE (10⁻¹K⁻¹) → 8.4

8. Thermal Conductivity (50 °C) → 15.4 W/m °C/ (300 K) → (21.9 W/mK)

9. Specific heat → 523 J kg⁻¹K⁻¹

10. Electrical Resistivity → 0.42 μΩm

11. The heat of Fusion (ΔH_m) → 3.7 kcal/m (14.15 kJ/mol)

12. Heat of Vaporization (ΔH_v) → 102.5 kCal/m (425 kJ/mol)

13. Heat of Transition (ΔH_t) → 0.950 kCal/m

14. Crystal structure → BCC, CPH

15. Corrosion Resistance → Very High

16. Reactivity with Oxygen → Very High

17. Atomic No. → 22

18. Modulus of elasticity → 105 GPa

19. Yield Strength → 692 GPa

20. Ultimate Strength → 785 GPa

21. Hardness (α -Ti, 700 °C Annealed) → 70HRB (Rockwell)

22. Bulk Modulus → 108.6–110 GPa

23. Specific gravity $\left(\frac{\text{sp. weight}}{\text{sp. weight of H}_2\text{O}} \right)$ → 4.5

24. Electrons per shell → 2, 8, 10, 2

25. Atomic radius → 147 pm

26. Young Modulus → 116 GPa

27. Shear Modulus → 44 GPa

28. Poisson ratio → 0.32

- 29. Mohs' Hardness → 6.0
- 30. Vickers Hardness → 970 MPa
- 31. Brinell Hardness → 716 MPa
- 32. Speed of sound → 5090 m/s
- 33. Magnetic ordering → Paramagnet
- 34. Covalent radius → 160 ± 8 pm
- 35. Oxide States → 4, 3, 2, 1 (amphoteric oxide)
- 36. Ionization energies:
 - 1st → 658.8 kJ/mol
 - 2nd → 1309.8 kJ/mol
 - 3rd → 2652.5 kJ/mol
- 37. Electronegativity → 1.54 (Pauling scale)
- 38. Half-life (^{44}Ti) → 63 year
- 39. Isotopes (6) → ^{44}Ti , ^{46}Ti , ^{47}Ti , ^{48}Ti , ^{49}Ti , ^{50}Ti
- 40. Crystal Structure → CPH

Ti α -phase → attributed to increase the strength i.e. properties

Ti β -phase → attributed to increase the corrosion resistance

14.2 Describe Properties of an advanced biomaterial (Niobium)²

- Group 5, Block → d, Transition metal
- 1. Atomic weight → 92.9 g/mol
 - 2. Atomic number → 41
 - 3. Atomic volume → $10.83 \text{ cm}^3/\text{atom}$
 - 4. Density → 8.57 g/cm^3
 - 5. Crystal Structure → BCC
 - 6. Coordination number → 8
 - 7. Electron configuration → $[\text{Kr}] 4d^4 5s^1$
 - 8. Electron per shell → 2, 8, 18, 12, 1
 - 9. Atomic radius → $1.46 \text{ \AA}^0$ (146pm)
 - 10. Melting Point → 2477°C
 - 11. Boiling Point → 4744°C
 - 12. The heat of Fusion (latent) → 30 kJ/mol

13. Latent Heat of Vaporization → 689.9 kJ/mol
14. Specific Heat (25 °C) → 24.6 J/mol K
15. The heat of Combustion → 2379 cal/g
16. Thermal Conductivity (300 K) → 53.7 W/mK
17. CTE (cm/cm/°C) → 7.88×10^{-6}
18. Electrical Conductivity → 152 nΩm
19. Young's modulus → 105 GPa
20. Shear Modulus → 38 GPa
21. Bulk Modulus → 170 GPa
22. Poisson ratio → 0.4
23. Mohs Hardness → 6.0
24. Vicker's Hardness → 1320 MPa
25. Brinell Hardness → 736 MPa
26. Speed of Sound (20 °C) → 3480 m/s
27. Oxidation States (mildly acidic oxide) → 5, 4, 3, 2, −1
28. Electronegativity → 1.6 (Pauling scale)
29. Covalent radius → 164 ± 6 pm
30. Ionization energy:
 - 1st → 652.1 kJ/mol
 - 2nd → 1380 kJ/mol
 - 3rd → 2416 kJ/mol
31. Magnetic ordering → Paramagnetic
32. Isotope (9) → ^{91}Nb , $^{91\text{m}}\text{Nb}$, ^{92}Nb , ^{92}Nb , ^{93}Nb , $^{93\text{m}}\text{Nb}$, ^{94}Nb , ^{95}Nb , $^{95\text{m}}\text{Nb}$
33. Half-life(^{91}Nb) → $6.8 \times 10^2 \text{ years}$

Footnotes

¹ Data are provided based on the reference, “Titanium”, Encyclopædia Britannica. 2006 and Samsonov, G. V. (1968). “Mechanical Properties of the Elements”. In G. V. Samsonov (ed.). Handbook of the physicochemical properties of the elements. New York, USA.

² Data are provided based on the reference, “Titanium”, Encyclopædia Britannica. 2006 and Samsonov, G. V. (1968). “Mechanical Properties of the Elements”. In G. V. Samsonov (ed.). Handbook of the physicochemical properties of the elements. New York, USA.

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15. Application to Biomaterials

Nabisab Mujawar Mubarak¹ , Mahmood Anwar² , Sujan Debnath³ 
and Izman Sudin⁴ 

- (1) Petroleum and Chemical Engineering, Faculty of Engineering, Universiti Teknologi Brunei, BE1410 Bandar Seri Begawan, Brunei Darussalam
- (2) Department of Mechanical Engineering, School of Computing, Engineering and Built Environment, Glasgow Caledonian University, Glasgow, Scotland, UK
- (3) Department of Mechanical Engineering, Curtin University Malaysia, Miri, Malaysia
- (4) Department of Materials, Production and Industrial Engineering, Faculty of Mechanical Engineering, Universiti Teknologi Malaysia, Johor Bahru, Malaysia

 **Nabisab Mujawar Mubarak (Corresponding author)**

Email: mubarak.mujawar@utb.edu.bn

Email: mubarak.yaseen@gmail.com

 **Mahmood Anwar**

Email: Mahmood.Anwar@gcu.ac.uk

 **Sujan Debnath**

Email: d.sujan@curtin.edu.my

 **Izman Sudin**

Email: izman@utm.my

15.1 Introduction

Biomaterials have been increasingly prevalent over the past few decades in the quickly developing pharmaceutical and medical industries. Biomaterials are substances used for medicinal and diagnostic purposes that are designed to interact with living biological tissue. Earlier, these materials were only used in medical devices to treat or replace tissue or improve organ functions. However, it was later discovered that the label “non-viable” used to describe them is incorrect because biomaterials have uses beyond just implanted devices. In diagnosing and treating many human diseases, biomaterials play a significant role in our everyday practice. In general, biomaterials are any materials—natural or artificial—that are biologically compatible with the human body and utilized to support, improve, restore, or replace the biological function of damaged tissues while coming into constant touch with bodily fluids.

A biomaterial is a substance developed to interact with biological systems for therapeutic (treating, enhancing, repairing, or replacing a tissue function of the body) or diagnostic purposes. Biomaterials have been a field of study for about fifty years. Biomaterials science or biomaterials engineering is the study of biomaterials. Throughout its history, it has grown consistently and strongly due to numerous businesses making significant financial investments in creating new products. The field of biomaterials science combines aspects of tissue engineering, biology, chemistry, and materials science. Be aware that a biomaterial is distinct from a biological material created by a biological system, such as bone. Additionally, caution should be taken when designing a biocompatible biomaterial because it depends on the application. While a biomaterial is friendly or appropriate for one application, it might not be in another.

15.2 What Are the Basic Features Required for the Biomaterial

Since the body tissues and bodily fluids are in direct touch with the biomaterials, some fundamental characteristics are necessary for the biomaterial, such as biocompatibility, inertness, safety, stability, cost-effectiveness, and ease of fabrication (see Fig. [15.1](#)).

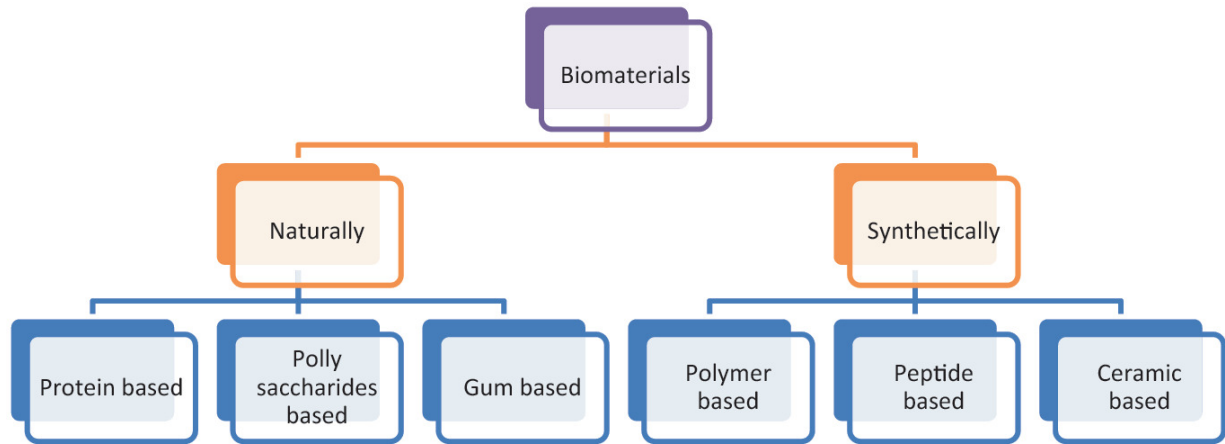


Fig. 15.1 Classification of biomaterials based on naturally and synthetically

15.3 Materials Used as Biomaterials

Biomaterials that can be further engineered using biochemical, biophysical, or biomechanical signals following the anticipated demands can be built using ceramics, metals, polymers, and composite materials.

15.3.1 Ceramics

Ceramics, often known as bio-ceramics, are biocompatible materials. While certain bio-ceramics are flexible, most are normally rigid materials used for surgical implants. The long-lasting metal oxides or the body's materials make up bio-ceramics. The ongoing advancements in biomaterials have increased the average duration range.

Due to their biocompatibility and mechanical qualities, inert ceramic materials were discovered to be employed for structural bone replacement in the 1950s. Because of how quickly they degrade, ceramic materials like glass–ceramic, bioactive glasses, calcium sulphates, and phosphates have been employed as bone grafts and for coating metallic implants since the 1980s. Later, it was discovered to host cells successfully and bioactive compounds on a ceramic scaffold to regenerate bone tissue. The creation of the implanted scaffolds can deliver antibiotics over an extended period. Bio-ceramic materials are utilized in biomimetic systems and are created to have mechanical and biophysical characteristics that match the original tissue's structure. The functions of these systems are intended to be similar to those of the original tissues, but they can be enhanced by integrating medicinal molecules. The biomimetic ceramics can load medicinal

compounds and improve protein absorption. Some biomimetic ceramics are also employed as medicinal molecules, such as glass, which has antibacterial properties. Ceramics can be divided into two categories: absorbable/non-inert and non-absorbable/non-inert (Alumina, zirconia, silicon nitrides, and carbons) (calcium phosphates and calcium aluminates). There are various generations of bioceramic materials, and each one contains a certain kind of substance.

15.3.2 Polymers

The mainstays created for the delivery of therapeutic medications are polymers. Since polymers can break down into bodily metabolites or be excreted from the body, they offer a wide range of applications in the biomedical area. Applications for polymeric biomaterials in the biochemical, biotechnological, medical, and pharmaceutical fields have been observed. Different strategies are used to synthesize various polymers. Wounded tissues are replaced using polymeric scaffolds (hard and soft tissues). Because of their subpar mechanical qualities, polymeric alternatives are less frequently used in hard tissue engineering. Thus, cross-linking via chemical processes is carried out to enhance the mechanical qualities.

Bioactive agents or pharmaceuticals are entrapped inside an insoluble matrix with sub-nanometer, nanometer, or micrometer-sized dimensions to offer regulated drug delivery. The most popular choice for a matrix for the regulated release of medicinal drugs is a polymeric material. Better drug integration, precise drug targeting, controlled drug release, improved stability, maximum distribution, and less toxicity while preserving therapeutic action are desired characteristics of a biodegradable polymer.

15.3.3 Natural Polymers

A marine polymer from red seaweed called agarose has a high level of bioactivity, thermogelling behavior, and switchable chemical reactivity for functionalization, among many other advantageous characteristics. Agarose is thus employed in creating numerous medication delivery systems as a therapeutic drug carrier. The brown algae *Laminaria hyperborea*, *Laminaria digitata*, *Laminaria japonica*, *Ascophyllum nodosum*, and *Macrocystis pyrifera* are the most often used sources of the biomaterial

alginate. Due to its strong mechanical attributes and appealing biological traits, nanocellulose has demonstrated considerable promise.

Due to its high molecular weight and hydrophilicity, pectin produced from plant cell walls is a perfect choice for hydrogel synthesis and 3D bioprinting. Fucoidan is a water-soluble polymer produced from marine brown algae. A polysaccharide found in cereals and tuber plants, starch is. A biomaterial called collagen is utilized to create scaffolds for the healing of wounds. Since it is the primary constituent of the dermal extracellular matrix, it is typically employed for skin wound healing because it is abundant in the body. Due to their release properties and stickiness, chitin and chitosan derivatives are polymeric materials utilized for various purposes, including excipient, drug carrier, oral mucoadhesive, and water-resistant adhesive.

15.3.4 Synthetic Polymers

Depending on the monomeric units, polyesters can be created from a number of monomers using the condensation and ring-opening polymerization processes. There are numerous synthetic development paths for polyesters. A synthetic polymer being studied for use in biomedical applications is polyglycolide. Due to its high degree of crystallinity, this polymer has poor solubility in organic solvents and a high tensile modulus. Due to its great crystallinity, it exhibits exceptional mechanical qualities. Compared to other biodegradable polymeric systems used in medicine, polyglycolide is very rigid.

One category of synthetic polymers is polycarbonate. They belong to a class of thermoplastic polymers with carbonate groups built into their structure. Aliphatic carbonates become pliable between 40 and 50 °C. Thermoplastic polyethylenes have a crystalline structure. It is described as an ethylene polymer made through addition polymerization, linear polymers, and condensation processes. Biomaterials based on polyphosphazene are a recently created biomaterial utilized in biomedicine. These unique polymers have extraordinary advantages that are not frequently encountered in other classes of polymers, such as poly(ϵ -caprolactone) and poly(lactic-co-glycolic acid). Although the polymer has not yet been fully utilized, it has demonstrated intriguing properties for tissue engineering and medication delivery.

15.3.5 Metals

Medical implants made of metal are quite important. Because of their mechanical qualities, biocompatibility, minimal friction, affordability, and resistance to corrosion, metallic biomaterials are favoured. However, they are quite aggressive to the microenvironment, which can result in metal oxidation and the release of undesired metallic ions, both of which can harm and inflame the local tissues. The most prevalent metallic biomaterials are steels, stainless steel, titanium alloys, cobalt-chromium alloys, gold, and gold alloys.

Metallic biomaterials offer a variety of inherent qualities, including strength, electrical conductivity, durability, mechanical dependability, and resistance to corrosion and wear. These characteristics of metallic biomaterials make metals more dominant than other materials in medical equipment. Nearly 70–60% of manufactured implants are discovered to be made of metal.

Iron and the synthesis of vitamin B-12 are two examples of metallic elements necessary for red blood cell activity but cannot be consumed in substantial quantities by the body. Because metallic biomaterials might corrode in an in vivo environment, their biocompatibility is a major concern. A variety of intrinsic physiological relevance, biocompatibility, and biodegradability are displayed by zinc as a metal biomaterial. Carbon nanomaterials are used for cancer treatment, drug delivery, and tissue engineering.

15.3.6 Composites

The term “composite” describes materials in which the elastic modulus qualities can be changed, and the defined phases are split on a scale larger than the atomic level. Wood, bone, dentin, skin, and cartilage are a few natural composite materials. One of the phases in foam as a composite is empty. Lung, cancellous, bone, and wood are examples of natural foams. The use of composite as a biomaterial applies to bone cement, dental filling composites, and orthopedic implants. Composites are generally more durable than any raw elements used to create them.

In contrast to metals and ceramics, which have drawbacks, including limited bioavailability and metal corrosion, composites have advantages. Recently, various diverse composite materials have been created for use in biomedical applications, and they are quickly rising to the top of the list for

use in load-bearing tissue components. The composite biomaterials are superior to ceramic materials in terms of fracture strength, high biocompatibility, and lack of corrosion.

Table 15.1 illustrates several biomaterial kinds’ benefits, drawbacks, and uses.

Table 15.1 Advantages, disadvantages and application of biomaterials

Types of biomaterials	Disadvantages	Advantages	Applications
Ceramics	Difficult manufacturing, low impact strength, reproducibility	Inert, corrosion resistance, high biocompatibility, low thermal and electrical conductivity	Surgical implants, dental parts, Coatings, structural bone replacement, medical equipment, bone fillings and bone tissue regeneration
Biocomposites	Difficult to reproduce during fabrication	Inert, corrosion resistant, superior biocompatibility	Heart valves, implants, knee implants and artificial joints
Metals	Mechanical properties differ from biological tissues with low biocompatibility and corrosion resistance in physiological environments	Ductility, high Mechanical resistance, low friction, low cost	Joint prostheses, dental implants
Polymers	Low mechanical resistance	Easy to Fabricate, low frictional properties	Implants, replacement of tissues, eye lenses, Sutures, and artificial tendons

15.4 Applications of Biomaterials

Figure 15.2 illustrates some of the many pharmaceutical and medical uses for biomaterials, including organ regeneration, medication delivery, tissue engineering, etc.

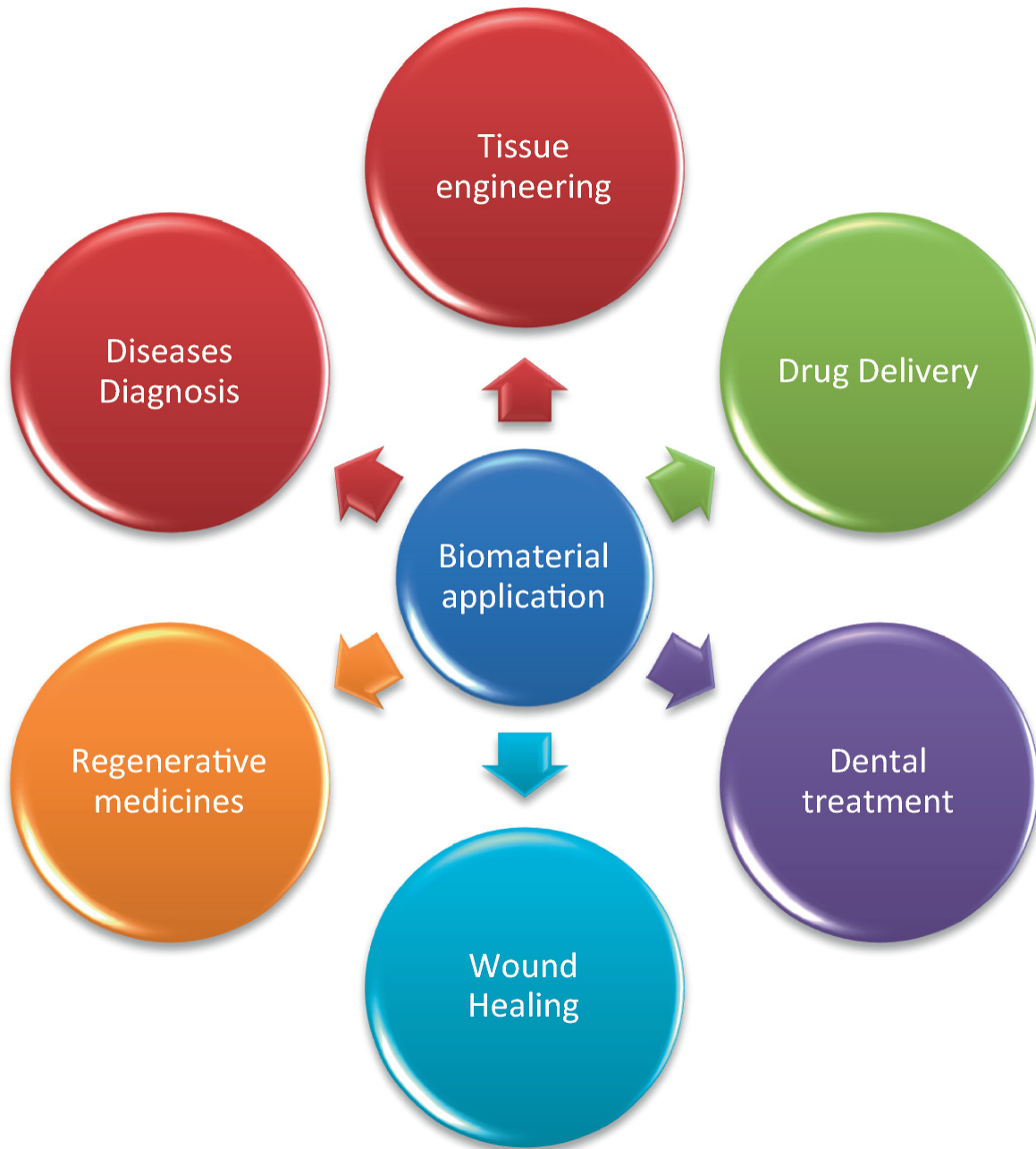


Fig. 15.2 Application of biomaterials

15.4.1 Dental Application

Dental biomaterials include substances such as resin composites, titanium alloys, zirconia, and others utilized in dentistry. Creating an entire tooth and tissues resembling dental pulp is possible. Using cultivated cells seeded on artificial extracellular matrices as a biomaterial, tissue engineering can be utilized to restore missing tissue. In the end, it was discovered that tooth

engineering is possible. By creating the nanoparticles, biomaterials for calcium hydroxide sustained release, such as chitosan or gelatin, were employed for root canal infections. The process of periodontal regeneration was carried out using an enamel matrix derivative, a protein-based biomaterial. The expression of markers for odontoblasts and odontoblast-like cells found in the human tooth pulpal tissue is also increased using derivatives of the enamel matrix. Injectable biomaterial scaffolds can be used to regenerate dental tissue. Various dental issues can be resolved by creating nanoparticles from polymeric biomaterials.

Organ Regeneration

Heart—Stem cells were attached to biomaterials to create a biocompatible cardiac patch, which was subsequently implanted. Cardiomyocytes embedded in hydrogel patches have been shown to exhibit contractile characteristics and mechanical stimulation.

Lungs—By seeding the pulmonary epithelium and vascular endothelium on rat decellularized scaffolds, lungs have been reconstituted *ex vivo*.

Knee—The two forms of ceramic-based functional biomaterials were proposed to prevent aseptic loosening during total knee replacement surgery and enhance the bone prosthesis system's functionality. Functionally graded biomaterials based on alumina and zirconia demonstrated excellent performance.

Tracheal graft—Various biomaterials, including hyaluronan poly(ethylene glycol), chitosan-collagen, collagen vitrigel membrane, fibrin glue, silk fibroin, and gelatin, have been used to create tracheal epithelial grafts. The disorders connected to the airways benefited from this. Engineering the organs can lead to the development of biomaterials that can replace the liver, kidney, airways, trachea, and larynx.

15.4.2 Regenerative Medicines

Regenerative therapies can be used to replace tissues that have been lost as a result of disease, trauma, or other abnormalities. Regenerative medicine uses interdisciplinary medical, material, and biological principles to enhance tissues and organs' biological makeup and functionality. Drug delivery and tissue engineering are combined. Regenerative medicine aims to implant scaffold materials for tissue regeneration. Cell scaffolds are

important because they function as an artificial extracellular matrix and a temporary home for the cell to be sustained.

In terms of biomaterials and regenerative medicine, urology is likewise evolving. Regenerative urology, initially used to repair small sections of the urinary system, has improved to the point that 3D models for complete functional organs are now accessible. Hyaluronic acid, which makes up the majority of the extracellular matrix in the brain, is used in CNS regenerative treatments because of its crucial role in understanding and managing CNS diseases. The biological activity and chemical modification of hyaluronic acid allows for the creation specialized and flexible scaffolds for CNS tissue engineering and regenerative medicine.

15.4.3 Tissue Engineering

Creating scaffolds is the key step in a successful tissue engineering process. The number of materials used in the construction must have been substantial. Numerous organic and synthetic polymers can be used to construct the scaffolds. Electrically conductive polymers can be used with other polymers to create improved biological and physiological properties when electric fields are applied during tissue engineering.

Electrospun nanofibers are used in several tissue engineering applications. Although electrospinning cannot be used to make scaffolds, it can be combined with 3D printing to produce electrospun nanofiber as a biomaterial and conveniently deliver cell stimulatory chemicals. Artificial organs can be created using tissue engineering. To maximize remodeling and functional outcomes for a particular development, the material's design, which includes the pore size and degradation kinetics, and the functionalization with cell- and tissue-specific components, the intrinsic factors of the tissue constructs, can be controlled.

15.4.4 Wound Healing

Silk has been used as a biomaterial to create silk grafts, promoting wound healing. Different biomaterials can be used for wound dressings and repair by electrospinning them into nanofibers. Biomaterials containing antioxidant capabilities have been shown to hasten the healing of chronic wounds. A bioactive glass composite biomaterial is utilized to speed wound healing. Important biomaterials for the recovery of wounds include chitin and chitosan. Itaconic acid was used in graft copolymerization on starch

and alginic acid in the presence of graphene sheets and Fe₃O₄ nanoparticles to form a magnetic composite hydrogel for guaifenesin, which was useful for drug delivery and wound healing. Protease-modulating products may be used to heal chronic wounds.

A great option for wound healing is hydrogel since it can act as a barrier between germs and the damp environment. Polyvinyl alcohol is frequently used to make hydrogel, which is used for wound healing. Calcium alginate hydrogel has been employed as a protamine drug carrier with neovascularization properties in treating chronic wounds. The skin-found polysaccharide hyaluronan is incredibly helpful as a hydrogel for wound healing. Hyaluronan and chitosan are combined to give vascular endothelial growth factor, which has antimicrobial and angiogenic characteristics and improves wound healing.

15.4.5 Drug Delivery

The rapid advancement of research and technology has led to the use of biomaterials in various sectors, including medicine, tissue engineering, biology, physics, and chemistry. Biomaterials have been studied and employed in pharmaceutical drug delivery over the past 50 years. They have been discovered to improve the distribution and efficacy of various therapeutic agents, including antibodies, peptides, vaccines, and enzymes. An-Yong Cai et al. claimed that biomaterials offer many benefits and are used to create nanocarriers with high drug loading capacities, strong biocompatibility, and good biodegradability. These nanocarriers are then employed for drug delivery. Drug delivery methods by synthetic biominerals that are well-designed Nanocarriers can aid in stopping drug leakage in the past and shield the drug from becoming inactive throughout circulation. Chemotherapeutic medicines, DNA, and proteins are delivered via biomineral-based nanocarriers. Drug delivery uses nanofibrous biomaterials because of their high potential and structural similarities to the extracellular matrix. Nanofibrous biomaterials can be created using a variety of natural and polymeric materials. The condition of neural cells and numerous extracellular components, which organize cellular behavior into appropriate tissue functions, are essential to the central nervous system (CNS) functioning. To increase or restore the function of extracellular components in the CNS in the event of injury and disease, biomaterials are essential. In addition to being used to distribute proteins or medications,

biomaterials are also employed for cell transplantation. Extracellular matrix components are becoming the source of biomaterials for engineering that can trigger desirable cell-specific responses. Hao Xing et al. have described using various biomaterials made from naturally occurring extracellular matrix proteins to control how cells function. Marco Corti et al. have created polyacrylate patches as a biomaterial for transdermal medication delivery using the high internal phase emulsion approach for wound healing. Utilizing mungbean starch and polyvinyl alcohol, Han-Seong Kim et al. created atenolol imprinted polysaccharide biomaterials and assessed their drug release characteristics.

15.4.6 Other Applications

Clinical applications of nanoscale metal–organic frameworks include cancer treatment and illness detection. To diagnose and treat Alzheimer's disease, a multifunctional nanoscale metal–organic framework-based nanoplatfrom was developed. 76 Radiation therapy is used to treat cancer but has some negative effects. Combining radiation and chemotherapy with biomaterials results in safer and more efficient therapy administration. Diagnostic imaging uses for biomaterials have changed, and they are also evolving in theranostics, combination therapy, and tissue protection. Non-biodegradable polymers, such as hydrogel implants, can be employed to preserve bioactivity in vivo while facilitating the prolonged release of anti-vascular endothelial growth factors. For various retinal illnesses, anti-vascular endothelial growth factors are now the preferred therapy option. For use as cardiovascular implants, poly-dopamine/hyaluronic acid coatings were produced on the NaOH passivated Mg-Zn-Y-Nd alloy. The functional impacts of absorption, immunomodulation and antibacterial activity on diabetic skin wounds have been demonstrated by cryogel/hydrogel biomaterials.

15.5 Conclusion

The most interdisciplinary field may be biomaterials. Since their development, they have demonstrated excellent use in the medical and pharmaceutical fields. The body uses many biomaterials kinds for various purposes. Implants made of different biomaterials can be used for organ regeneration, tissue engineering, wound healing, disease diagnostics, drug

delivery, and simulating the structure and function of tissues and organs. Recently, urology and cell regeneration have both shown use for biomaterials. In addition to various drug delivery scaffolds, nano-carriers play a significant role in drug delivery. In the pharmaceutical and medical industries, biomaterials play an increasingly important role.

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